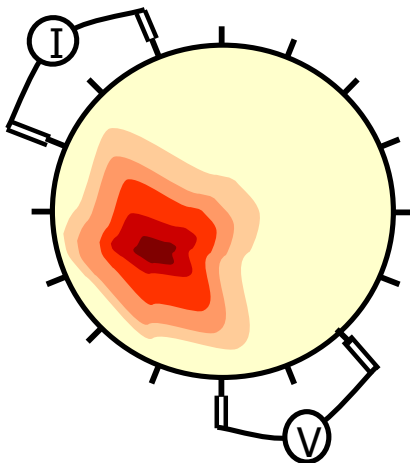
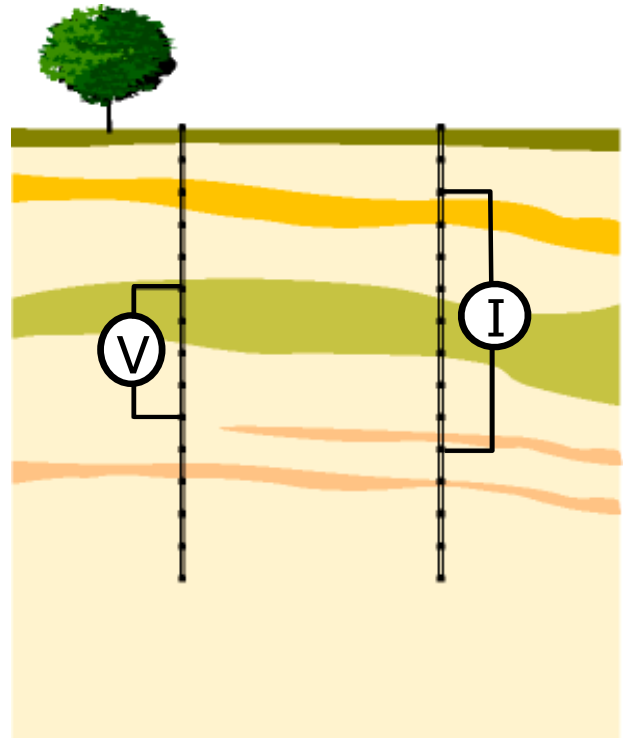
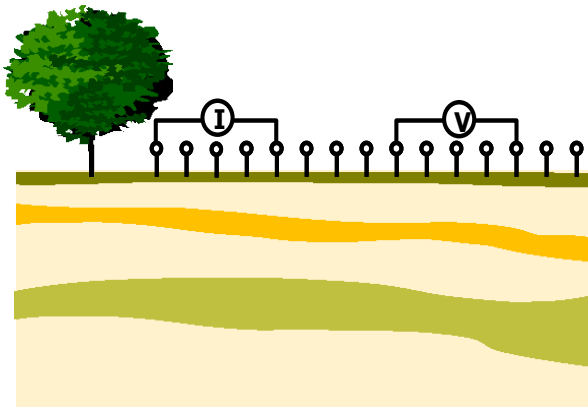
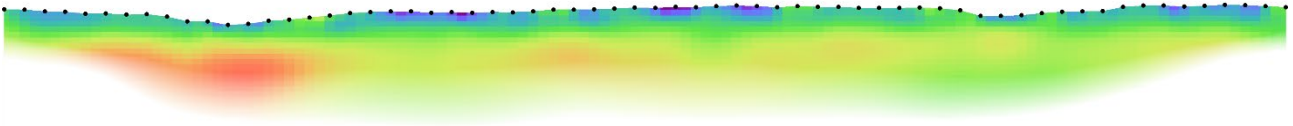

R2

version 4.11 (September 2023)

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September 2023



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1. Recent version history

Changes to *R2* from v4.10

Minor bug fixes.

Changes to *R2* from v4.02

Sensitivity map output now also includes a value scaled by parameter cell area. Additions to documentation made.

Changes to *R2* from v4.01

If the starting model satisfies the data then output is generated (previously the files were left empty).

Bug fix: output of estimate of memory required corrected.

Changes to *R2* from v4.0

The calculation of resolution matrix has been improved. Checks for vtk output of negative values of resolution matrix made. Minor edits to output and documentation.

Changes to *R2* from v3.3

General quadrilateral mesh input now an option. When a triangular mesh is used the mesh.dat file now needs specification of the Dirichlet node in line 1. Bug fix: difference inversion file output now corrected.

Error checking on presence of input files. Mesh error checks when mesh is read from file **mesh.dat**.

Output of model roughness in main log file.

Changes to *R2* from v3.2

Bug fix: geometric factor calculations for triangular meshes. Bug fix: output of electrode codes in the _err.dat file (only has impact if electrode numbers are different to the order they are defined in **R2.in**).

Bug fix: incorrect step length set when convergence reached in first alpha trial.

Changes to *R2* from v3.1

Bug fix: calculations with a triangular mesh when node 1 was close to (or at) an electrode (that resulted in high errors in forward model calculations for measurements involving such an electrode).

In a difference inversion the vtk output file now contains the percentage differences. Error checks on input of the data file (**protocol.dat**) are now made (to avoid incorrect electrode numbering). Output of a vtk file containing inversion results at each iteration is now included (previously this was only output to a **.dat** file). Some utility codes have been added to help with creating triangular meshes. Third party codes and scripts have been added. Documentation has been improved by adding more illustration of meshing and parameterisation.

Changes to *R2* from v3.0

Anisotropic regularisation is now implemented for a triangular mesh. In earlier versions anisotropic regularisation only worked for quadrilateral meshes. An example triangular mesh problem is included in the distribution and this document. In addition, the output of co-ordinates of the mesh has changed for a triangular mesh (the polarity of the vertical co-ordinate) to allow some consistency with quadrilateral mesh problems and some notes are added in this document about co-ordinate conventions.

Changes to *R2* from v2.7c

All main arrays are now set at run time and so there is no set limit to the size of the problem that can be solved. Because *R2* can now work with much larger problems the forward solver uses pardiso (e.g. <http://www.pardiso-project.org/>) as a linear equation solver, which allows more compact array storage. Users may find that smaller problems run a little slower than with earlier versions because of the overheads in using this solver. *R2* now also allows more control of the convergence by specifying a target decrease in misfit at each iteration (see changes to entry of Line 18 in **R2.in**).

Changes to *R2* from v2.7b

Option to output roughness matrix and Jacobian.

Changes to *R2* from v2.7a

Bug fix for input of poly line specifying output region. Note that example files supplied for v2.7a and earlier will not output the region properly with 2.7b – these input files have been changed with this release. Also changed upper limits of problem size.

Changes to *R2* from v2.7

Bug fix for case when parameter number set to zero.

2. Computer requirements for **R2** v4.11

In this release two versions have been compiled for the Windows environment. A 64bit version, **R2.exe**, is provided in the package, along with the 32bit version (**R2_w32.exe**). The 32bit version is only provided for continuity of **R2** and its use is not recommended and it has not been tested. Linux and Mac users should be able to run **R2** with the command “wine R2.exe” (thanks to Rodolphe Cattin for this tip).

NOTE 1: ***R2** is provided as a standalone executable. It does not need to be installed – the executable is put in the folder containing the input files and run from there. Output files will be created in the same folder.*

NOTE 2: *You will be able to run **R2** by double clicking the executable. However, if the program stops abruptly (for example, due to an error in the input file or if you are trying to run an executable compiled for a different processor architecture) then you will not see any error message on the screen since the window will disappear. Therefore, it is advisable to run **R2** from the Command Prompt in Windows (just run CMD from the Start Menu – you may need to move your working directory and run **R2** from there).*

NOTE 3: *All input files should be prepared with a text editor. [I prefer to use TextPad (<https://www.textpad.com/home>) because it allows much greater editing facilities although any text editor will work]. It is important that you do not include tabs in the files. These are often inserted if you copy and paste from Excel, for example. You should convert these tabs to spaces (TextPad will allow you to set this up to happen automatically).*

R2 has been designed so that no other commercial software is required for pre- and post-processing. Simple structured meshes can be created directly in **R2**, alternatively more complex geometry can be meshed using freely available codes, such as **Gmsh** (<https://gmsh.info/>). **R2** does not produce graphical output but results compatible with the freely available **ParaView** (<https://www.paraview.org>) are produced. Other free codes, such as **GMT** (<https://github.com/GenericMappingTools/gmt>) can be used. Users wishing to use a graphical user interface for meshing, modelling and plotting may be interested in **ResIPy** - an open source python GUI for **R2** and sister codes. See <https://gitlab.com/hkex/resipy> which also includes links for standalone executables. Video tutorials for **ResIPy** are available at <https://www.youtube.com/c/ResIPy>. See also Boyd et al.(2019) and Blanchy et al.(2020).

3. Introduction to **R2** v4.11

R2 is a forward/inverse solution for 3D or 2D current flow in a quadrilateral or triangular mesh. The mesh is made up of a set of elements. Parameters (for the inverse solution) are made up of one or more elements. Electrodes are specified at node points. These are the corners of the elements. The boundary conditions along all four boundaries of the mesh are Neumann conditions (zero flux) and therefore if you are investigating a half space you must extend left, right and lower boundaries of the mesh to some distance away from the area of investigation (typically 5 to 10 times the distance – see later). One of the nodes must be set to a Dirichlet node (see later). The mesh can be made up of either quadrilateral elements or triangular elements.

The current version does not have upper limits set for the size of the problem that can be solved. However, it is important that the user has some appreciation of whether the problem they are trying to solve is realistic for their given hardware. Large problems in inverse mode can be memory hungry. As soon as the user's RAM is used then the computer will start using virtual memory (paging to disk) which can be very slow. To help the user assess memory needs **R2** will output an estimate of the memory needs early on in its execution. For large problems it is important that the user compares this with physical memory (RAM) that is available.

For information on **R2**, along with in-depth explanation of the theory behind forward and inverse modelling, see Binley and Slater (2020). Binley (2015) and Binley and Kemna (2005) also provide useful summaries of the theory underpinning **R2**. Contact the author for a digital copy of Binley (2015).

R2 is provided for non-commercial use. Any users wishing to use **R2** for commercial applications should contact the author.

DISCLAIMER

R2 has been used for a wide variety of applications and continues to be developed. It has been thoroughly tested, however, the user must accept all responsibility for the results and interpretation of the code's output. The author and Lancaster University provide no warranties to the user, expressed, implied, or statutory, including any implied warranties of fitness for a particular purpose. In no event will the author or Lancaster University be liable for any damages, including direct, indirect, special, incidental, or consequential damages, arising out of anyone's use of or inability to use this code.

4. Forward and inverse modelling in **R2**

4.1 Forward modelling

Forward modelling is used to determine transfer resistances (or apparent resistivities) for a given set of four electrode measurements and a given distribution of resistivity. It can be carried out explicitly in **R2** in forward mode, or used implicitly in **R2** in inverse mode. **R2** solves the governing equations using the finite element method.

We can write a 2D form of the governing equation (with x horizontal and y vertical) and resistivity, ρ , varying in x and z but constant in the third dimension, y , as:

$$\frac{\partial}{\partial x} \left(\frac{1}{\rho} \frac{\partial V}{\partial x} \right) + \frac{\partial}{\partial z} \left(\frac{1}{\rho} \frac{\partial V}{\partial z} \right) = -I \delta(x) \delta(z), \quad (1)$$

however, this assumes that the current source is infinitely long in the y direction, and so of limited practical value. To account for point electrodes we must account for 3D current flow (whilst assuming 2D variation in resistivity). To do this we can use the Fourier cosine transformation:

$$v(x, k_w, z) = 2 \int_0^\infty V(x, y, z) \cos(k_w y) dy, \quad (2)$$

where k_w is the wavenumber. This allows us to form a 2D equation in terms of the transformed variable, v as:

$$\frac{\partial}{\partial x} \left(\frac{1}{\rho} \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial z} \left(\frac{1}{\rho} \frac{\partial v}{\partial z} \right) - \frac{v k_w^2}{\rho} = -I \delta(x) \delta(z). \quad (3)$$

Equation 3 can then be solved for v , for a given value of k_w , in a 2D manner. To determine the voltage V , the inverse Fourier transform is needed. This can be stated as:

$$V(x, y, z) = \frac{1}{\pi} \int_0^\infty v(x, k_w, z) \cos(k_w y) dy, \quad (4)$$

which can be approximated with numerical integration. In **R2** this is done with a combination of Gaussian quadrature and Laguerre integration. To determine the voltage at the potential electrodes we, therefore, solve the 2D problem in equation 3 for a given number of values of k_w and then approximate V through equation 4.

As stated earlier, **R2**, solved the forward problem with the finite element method. With this method, the region of interest is discretised into a mesh of either 3 node triangular or 4 node quadrilateral elements and voltages computed at the node points of each element. Quadrilateral elements make mesh building easy but are less efficient computationally than triangular elements. Section 5 explains how meshes can be constructed.

As the finite element method approximates the governing equation we need to ensure that we do not create significant numerical discretisation errors – close to the electrodes the elements need to be finely discretised to ensure that a suitable accuracy is achieved. We can improve the accuracy of the forward modelling with *singularity removal*, this effectively decouples the problem into a primary and secondary voltage (see Lowry et al., 1989) using a known analytical solution for the primary voltages. **R2** allows singularity removal to be applied (see section on **R2.in** input for details) but the user must ensure that the region is an infinite half space with a flat surface, otherwise the analytical solution for the primary voltage will be incorrect.

4.2 Inverse modelling

In **R2** an iterative process solves the following equations:

$$(\mathbf{J}^T \mathbf{W}_d^T \mathbf{W}_d \mathbf{J} + \alpha \mathbf{R}) \Delta \mathbf{m} = \mathbf{J}^T \mathbf{W}_d^T (\mathbf{d} - \mathbf{f}(\mathbf{m}_i)) - \alpha \mathbf{R} \mathbf{m} \quad (5)$$

$$\mathbf{m}_{i+1} = \mathbf{m}_i + \Delta \mathbf{m}, \quad (6)$$

where:

\mathbf{J} is the Jacobian, such that $J_{i,j} = \partial d_i / \partial m_j$,

\mathbf{d} is the data vector,

\mathbf{m}_i is the parameter vector at iteration i ,

\mathbf{W}_d is the data weight matrix, assumed to be diagonal, with diagonal values $W_{d,i,i} = 1/\epsilon_i$, where ϵ_i is the standard deviation of measurement i ,

α is the regularisation (or smoothing) scalar,

\mathbf{R} is the roughness matrix, which describes the connectivity of parameter blocks,

$\Delta \mathbf{m}$ is update in parameter values at each iteration,

$\mathbf{f}(\mathbf{m})$ is the forward model for parameters \mathbf{m} .

In **R2** the parameters are the logarithm of the electrical conductivity in each element (or group of elements that form a parameter block). The data are either transfer resistances or, if log data selected (see detailed input instructions later for **R2.in**) then the input data are transformed to logarithm of transfer resistances. Note that this does not require only positive data, however, the forward model computed value should be the same polarity, otherwise the difference is not defined. If **R2** encounters a difference in polarity between modelled and measured values during an inversion then these measurements are ignored.

Equations 5 and 6 are solved repeatedly until satisfactory convergence is achieved. In **R2** this is defined by the data misfit reaching a required tolerance. If we express data misfit as a root mean square error, i.e.

$$\text{RMS} = \sqrt{\frac{1}{N} \sum \left(\frac{d_i - f_i(\mathbf{m})}{\epsilon_i} \right)^2}, \quad (7)$$

where N is the number of measurements, then the target tolerance should be 1 (following a chi-squared distribution).

Equations 5 and 6 result from the minimisation of an objective function composed of a data misfit and a model misfit. The former describes the mismatch between the observations (\mathbf{d}) and the forward model ($\mathbf{f}(\mathbf{m})$) and can be expressed as:

$$\Psi_d = (\mathbf{d} - \mathbf{f}(\mathbf{m}))^T \mathbf{W}_d^T \mathbf{W}_d (\mathbf{d} - \mathbf{f}(\mathbf{m})). \quad (8)$$

The model misfit describes the roughness of the variation in model parameter and can be expressed as:

$$\Psi_m = \mathbf{m}^T \mathbf{R} \mathbf{m}. \quad (9)$$

In an Occam's inversion we seek to minimise:

$$\Psi_{total} = \Psi_d + \alpha \Psi_m, \quad (10)$$

for the largest α , i.e. we wish to obtain the smoothest distribution of resistivity that is consistent with the observed data. **R2** achieves this through an iterative process in which equation 5 is solved and equation 6 applied. At each iteration α can change, keeping it as large as possible. **R2** does a line search for α at each Gauss Newton iteration (using up to 10 values of α). **R2** computes a reasonable starting value for α at the beginning of the process by assessing an equal balance of the terms in the brackets of left hand side of equation 5. This often results in satisfactory convergence within a few iterations.

However, this can lead to unsmooth models as the inversion process is attempting to find a solution too quickly. Sometimes it can be beneficial to slow the process. To do this the user can select the maximum change in misfit during each iteration (using the `target_decrease` parameter – see **R2.in** input). The user is recommended to experiment with either solution strategies. Note also that R2 allows the regularisation scalar, α , to be anisotropic in order to enhance smoothing in one direction.

During each iteration **R2** will output values of Ψ_d (reported as a root mean square (RMS) error) and Ψ_m (reported as “roughness”).

R2 allows different forms of the roughness matrix **R** in equation 5. This is achieved with the `inverse_type` parameter in **R2.in** (see section on **R2.in** input). Normally `inverse_type` is set to 1, which leads to a model misfit in equation 5 that is equivalent to the sum of squared differences between each parameter and adjacent parameter values (see Binley and Slater (2020) for more details). If `inverse_type` is set to 0 then a pseudo Marquardt inversion is carried out using a diagonal form of **R**, i.e. there is only damping but no spatial regularisation. This is unlikely to lead to a satisfactory convergence as is only included to maintain consistency with historic forms of **R2**. If `inverse_type` is set to 2 then greater smoothing is applied using the structure of roughness matrix **R**. Again this is only included for consistency with historic forms of **R2**. If `inverse_type` is set to 3 then a *qualitative* solution is computed. This is based on the weighted back projection method of Kotre (1994). It has shown some value for circular electrode arrays but it is unlikely to be of general value and should be avoided (the back projection approach was developed to allow rapid computation of an image but nowadays a normal 2D inversion can be achieved quickly). If `inverse_type` is set to 4 then the regularisation can be set so that some of the smoothing is switched off between adjacent parameter cells (see section on **R2.in** input). Note also, that some parameter cells can be forced to remain unchanged from the initial model specified by the user.

In addition to setting `inverse_type`, the user can control other aspects of the regularisation with the parameter `reg_mode` in **R2.in** (see section on **R2.in** input). The approach described above is achieved by setting `reg_mode=0` in **R2.in**.

In some cases we may wish to obtain a model that is smooth in terms of the difference between model parameter and some reference model. Such a situation is useful for time-lapse inversion (see later). In this case we could express a model misfit as:

$$\Psi_m = (\mathbf{m} - \mathbf{m}_0)^T \mathbf{R} (\mathbf{m} - \mathbf{m}_0), \quad (11)$$

where \mathbf{m}_0 is the reference parameter model.

An alternative regularisation (used in **R2** with `reg_mode=1`) is to use a model misfit as:

$$\Psi_m = (\mathbf{m} - \mathbf{m}_0)^T \mathbf{R} (\mathbf{m} - \mathbf{m}_0) + \alpha_s (\mathbf{m} - \mathbf{m}_0)^T (\mathbf{m} - \mathbf{m}_0), \quad (12)$$

where α_s is a weighting factor: a high value forces consistency with the reference model; a low value forces smoothing of the difference. In **R2** this is referred to as a *background regularisation*.

Alternatively we can consider the *difference inversion* approach of LaBrecque and Yang (2001), which has proved to be useful for time-lapse data. For this approach equation 5 needs to be modified to:

$$(\mathbf{J}^T \mathbf{W}_d^T \mathbf{W}_d \mathbf{J} + \alpha \mathbf{R}) \Delta \mathbf{m} = \mathbf{J}^T \mathbf{W}_d^T (\mathbf{d} - \mathbf{f}(\mathbf{m}_i)) - \alpha \mathbf{R} (\mathbf{m} - \mathbf{m}_0). \quad (13)$$

with the term:

$$(\mathbf{d} - \mathbf{f}(\mathbf{m}_i)) \quad (14)$$

defined as:

$$(\mathbf{d} - \mathbf{d}_0) - (\mathbf{f}(\mathbf{m}_i) - \mathbf{f}(\mathbf{m}_0)). \quad (15)$$

To implement this the user should set `reg_mode=2` in **R2.in** (see section on **R2.in** input) and provide two columns of data in **protocol.dat**: the first column is \mathbf{d}_0 , the second column is \mathbf{d} . **R2** uses these to create a new dataset:

$$(\mathbf{d} - \mathbf{d}_0 + \mathbf{f}(\mathbf{m}_0)), \quad (16)$$

where $\mathbf{f}(\mathbf{m}_0)$ is the forward model with the reference dataset \mathbf{d}_0 .

4.3 Inverse model appraisal

R2 provides two direct ways to assess the final model from an inversion. One approach for model appraisal, which is widely appreciated in general inverse theory, is the model resolution matrix, \mathbf{R}_m , which describes the mapping of data and model space, and is defined by:

$$\mathbf{m} = \mathbf{R}_m \mathbf{m}_{\text{true}}, \quad (17)$$

where \mathbf{m} is the inverted parameter set and \mathbf{m}_{true} is the (unknown) true parameter set. Clearly, ideally $\mathbf{R}_m = \mathbf{I}$, any deviation reveals the lack of sensitivity of the parameter values to the measured data, manifested by regularisation.

From the formulation in equation 17, \mathbf{R}_m can be approximated by the solution of:

$$(\mathbf{J}^T \mathbf{W}_d^T \mathbf{W}_d \mathbf{J} + \alpha \mathbf{R}) \mathbf{R}_m = \mathbf{J}^T \mathbf{W}_d^T \mathbf{W}_d \mathbf{J}, \quad (18)$$

where the Jacobian, \mathbf{J} , has been computed using the final (inverted) parameter set and the regularization scalar, α , is the value at the end of the inversion. The determination of \mathbf{R}_m using equation 18 requires significant computational effort: the formation and solution of M sets of equations, each of size $M \times M$, where M is the number of parameters. The simplest way to use the resolution matrix is to display the diagonal value for each parameter, which should be unity for perfectly resolved parameters – this is what is output if `res_matrix = 2` is specified in **R2.in** (see **R2.in** input section).

An alternative (and much easier computationally) way of assessing the inverse model is to use a sensitivity map. This is done by computing the diagonal of:

$$\mathbf{S} = \mathbf{J}^T \mathbf{W}_d^T \mathbf{W}_d \mathbf{J}, \quad (19)$$

i.e. for each parameter cell, j :

$$S_j = \sum_{i=1}^N (J_{i,j} W_{d,i})^2, \quad (20)$$

where N is the number of measurements.

To do this `res_matrix = 1` is specified in **R2.in**.

R2 will also output a scaled form of the value in equation 19 using the area of each parameter cell. This can be particularly useful if your mesh has significant variation in element sizes within the region of interest.

$$S_{s,j} = \sum_{i=1}^N (J_{i,j} W_{d,i} / A_j)^2, \quad (21)$$

where A_j is the area of parameter cell j .

In addition to these, other approaches are available for model appraisal, e.g. the depth of investigation approach of Oldenburg and Li (1999), the use of which is illustrated in one of the examples provided.

5. Designing meshes

R2 uses a mesh of finite elements to compute the forward model (in both forward and inverse mode). As stated earlier, the mesh is based on a quadrilateral (*structured* or *unstructured*) or triangular (*unstructured*) mesh of finite elements. Each element is defined by node points on its perimeter (see Figure 5.1). **R2** computes the voltage at each node point given a dipole current source applied at a pair of nodes. Therefore, the minimum requirement of the mesh is that the electrodes must be sited at node points. The accuracy of the computed voltage field is strongly dependent on the discretisation of the nodes: nodes should be closely spaced near electrode sites as voltage gradients will be high.

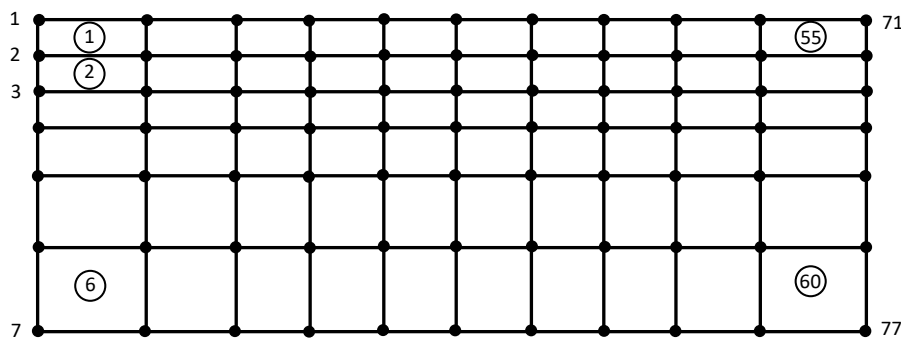


Figure 5.1: Example finite element showing ordering of nodes and elements (in circles) for a structured quadrilateral mesh. For unstructured meshes the user defines the element and node numbering.

The mesh should clearly cover the survey area laterally and the expected depth of investigation, however, given that injected current will transfer further horizontally and vertically, the mesh should extend sufficiently in order to account for this (mimicking infinite boundaries). There is no need to retain a fine discretisation in these ‘infinite’ boundary regions: it is good practice to let the elements gradually increase in size laterally and vertically outside the region of investigation. Figure 5.2 illustrates the zoning of discretisation. Note that this example is for a surface electrode array. For others, e.g. cross-borehole, similar concepts are applied.

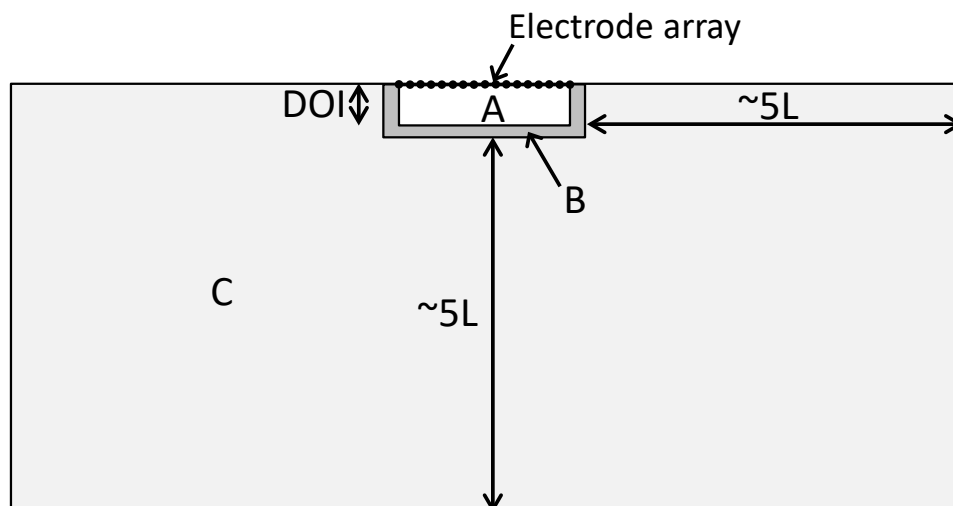


Figure 5.2: Extending the finite element mesh to account for ‘infinite’ boundaries. DOI is the depth of investigation. Zone A is the region of interest; elements should be finely discretised especially near the electrodes. Zone B has the same discretisation as A and is included to ensure good accuracy of the forward calculations; this zone typically extends two or three times the electrode spacing. Zone C typically extends $\sim 5L$ where L is the length of the longest current dipole. Discretisation should gradually get coarser in Zone C, moving away from the region of investigation.

A basic (structured) quadrilateral mesh in **R2** is defined by a grid of `numnp_z` rows and `numnp_x` columns of nodes. This type of mesh can be set in three different ways (Figure 5.3). The simplest type is a rectangular grid (Figure 5.3a). In **R2.in** we define this as `mesh_type = 4` (see later). In this case, the elevation of all nodes in a given row is constant. The mesh is defined by the x co-ordinates of each column, the z co-ordinates of the nodes in the top row (i.e. the topography) and the depth of each row relative to the top row. If the topography varies across the survey area then a mesh shown in Figure 5.3b results. Again this is `mesh_type = 4`. A more complex mesh structure (see Figure 5.3c) can also be created. In **R2.in** we define this as `mesh_type = 5`. In this case the x co-ordinates are still fixed for each column but the elevation of all nodes in each column must be input. In comparison to `mesh_type = 5` more input defining the geometry is needed but the co-ordinates of every node is not needed.

The basic (structured) meshes described above are generated by **R2** following input of geometrical parameters in **R2.in**. A more sophisticated (unstructured) quadrilateral mesh (e.g. Figure 5.4) can also be used in **R2** but this must be read from a separate file **mesh.dat** (`mesh_type = 6`). The file will contain the co-ordinates of all nodes, along with the element definitions (i.e. the four node numbers for each element). The specific format of **mesh.dat** is defined later.

For more complex geometry **R2** allows the use of a triangular mesh. Again, the co-ordinates for all nodes must be defined, along with the element definitions (i.e. the three node numbers for each element). In **R2.in** we define this as `mesh_type = 3` and the mesh is read from the file **mesh.dat**.

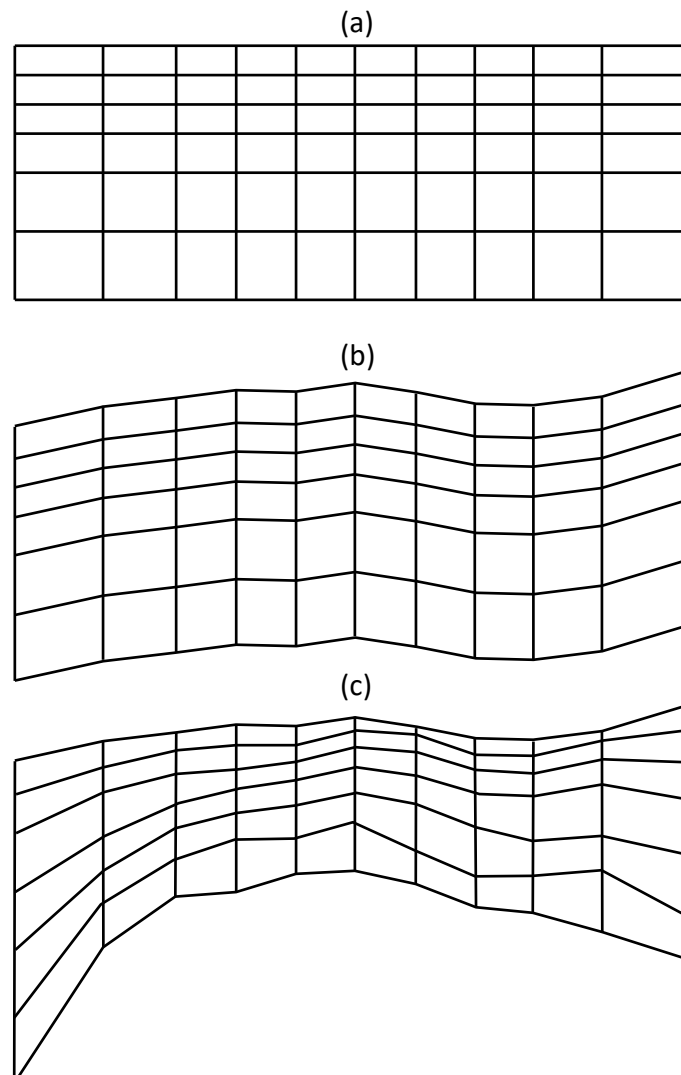


Figure 5.3: Basic (structured) quadrilateral mesh types. (a) and (b): `mesh_type = 4`; (c): `mesh_type = 5`.

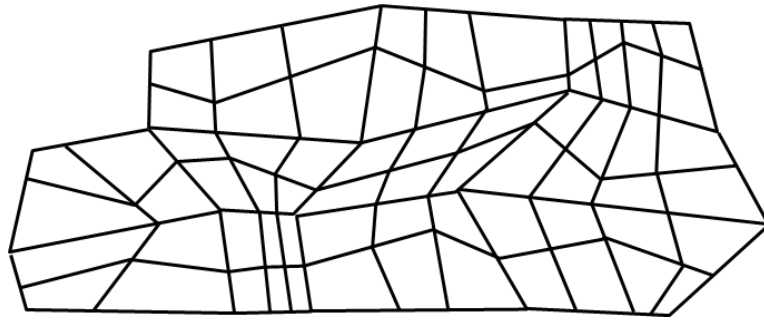


Figure 5.4: Unstructured quadrilateral mesh example (`mesh_type = 6`).

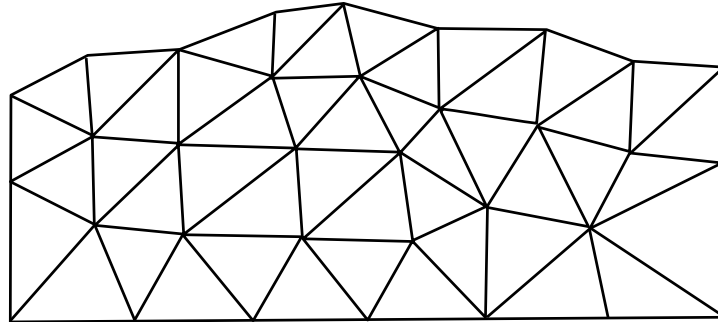


Figure 5.5: Triangular mesh example (`mesh_type = 3`).

If full flexibility in mapping the geometry of the problem is required then a triangular mesh is preferred. In some instances the use of a pre-defined quadrilateral mesh (`mesh_type = 6`) may be effective. It doesn't need to be unstructured. Figure 5.6 shows an example where rectangular geometry is used but since the mesh cannot be defined as one set of rows and columns, the mesh must be predefined and read from **mesh.dat**.

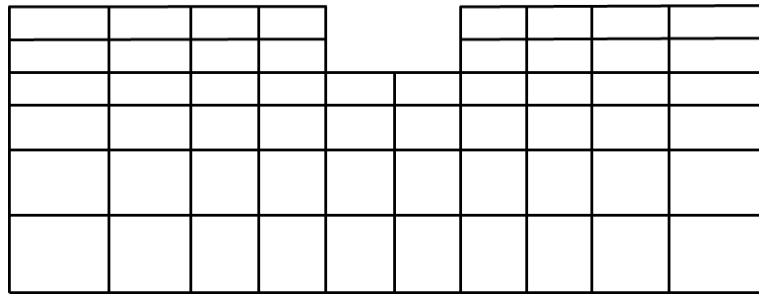


Figure 5.6: Structured quadrilateral mesh example (`mesh_type = 6`).

Triangular meshes not only allow full flexibility in defining geometry but also result in more computationally efficient meshes since the extremities of the mesh can be made to have coarser discretisation (see Figure 5.7). If you are working with a triangular mesh then you must create the mesh and store details of the geometry of the mesh in a file **mesh.dat**. There are a number of good meshing tools available. *Gmsh* (see <http://www.gmsh.info>) is a powerful finite element mesh generator with a large user base with video tutorials available online. Alternatively, software for general finite element analysis (e.g. *COMSOL*) contain mesh generators, as do software for specific applications (e.g. groundwater code environments like *GMS*).

A key constraint of the structured meshes (`mesh_type = 4` or `5`) is that defining the geometry of parameter cells in an inverse solution is constrained (see section 5). If the mesh is prepared in **mesh.dat** (`mesh_type = 3` or `6`) the user has full control of parameter discretisation and zoning (see later).

5.1 Gmsh mesh utility codes for *R2*

The *R2* download package contains some simple codes for working with *Gmsh*. These are located in the **Mesh_utilities/Binley** folder. *GenGmshGeo2D* creates a geometry file for *Gmsh*. This can then be loaded in *Gmsh* and a 2D mesh easily created. The mesh in *Gmsh* is saved as a file **GenGmshGeo2D.msh** which can be transformed to the **mesh.dat** format for *R2* using the partner code *GmshMsh2R2*. Note that Gmsh v3.0.6 was used in generating these scripts. More recent versions may not be compatible.

An important thing to note with mesh generation is that all finite elements should have node numbers in a counter-clockwise direction. I have noticed that *Gmsh* can produce mesh output with element nodes ordered in a clockwise direction. *R2* now includes a check on this and will fix ordering errors. *R2* will also check if duplicate nodes exist in the mesh (more than one node with the same coordinates). If these are found *R2* will report them and terminate – the user must then rectify the errors in the mesh file.

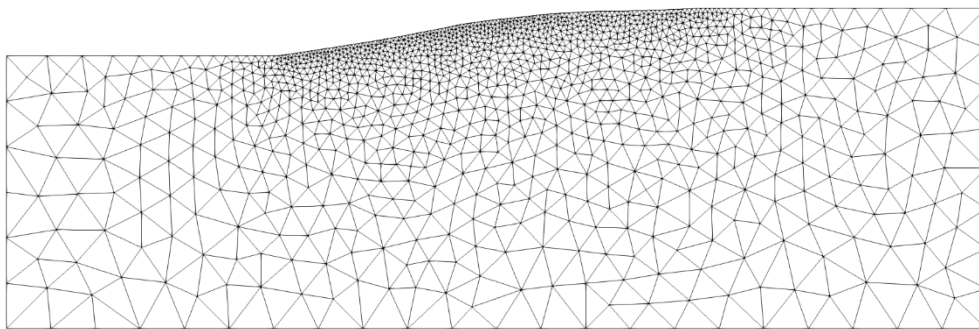


Figure 5.7: Example triangular mesh with variable discretisation.

Niels Claes (University of Wyoming) has provided a Matlab script (see folder **Mesh_utilities/Claes**) that will create a mesh file using *Gmsh*.

Jimmy Boyd (British Geological Survey/ Lancaster University) has written a python script to convert Gmsh msh files to **mesh.dat** format for *R2*. See **Mesh_utilities/Boyd**

Additionally, the graphical software *ResIPy* (<https://gitlab.com/hkex/resipy>) allows mesh generation within its interface of quadrilateral and triangular mesh.

Again, note that these scripts have been produced with specific versions of *Gmsh* and may not be compatible with more recent versions. Also note that the author has not tested these third party scripts.

6. Parameterisation

For a forward model calculation the resistivity for each element must be defined. For an inverse solution the starting resistivity model must be defined. This is normally a uniform model. In inverse mode the discretisation of parameters must be set. The simplest way to do this is to set each finite element as a parameter. In some cases a more complex parameterisation is required. In a structured quadrilateral mesh we can define 'patch' sizes for parameters. A patch is a group of elements, which is illustrated in Figure 6.1. The advantage of such patching of elements is the reduced computational time, since the number of parameters is reduced.

In some instances we may wish to fix the resistivity in part of the mesh, i.e. the parameters may only cover a subset of the finite element mesh (see, for example, Figure 6.2). **R2** allows this type of parameterisation by stating where the patching starts and ends in both x and y direction.

Greater control of parameterisation is allowed when a mesh is prepared *a priori*, for either a triangular mesh or a quadrilateral mesh (e.g. Figure 6.3) by defining a parameter number for each element in **mesh.dat**. Note that if a parameter number 0 is assigned for an element then the inverse solution fixes the resistivity of this element to the starting value.

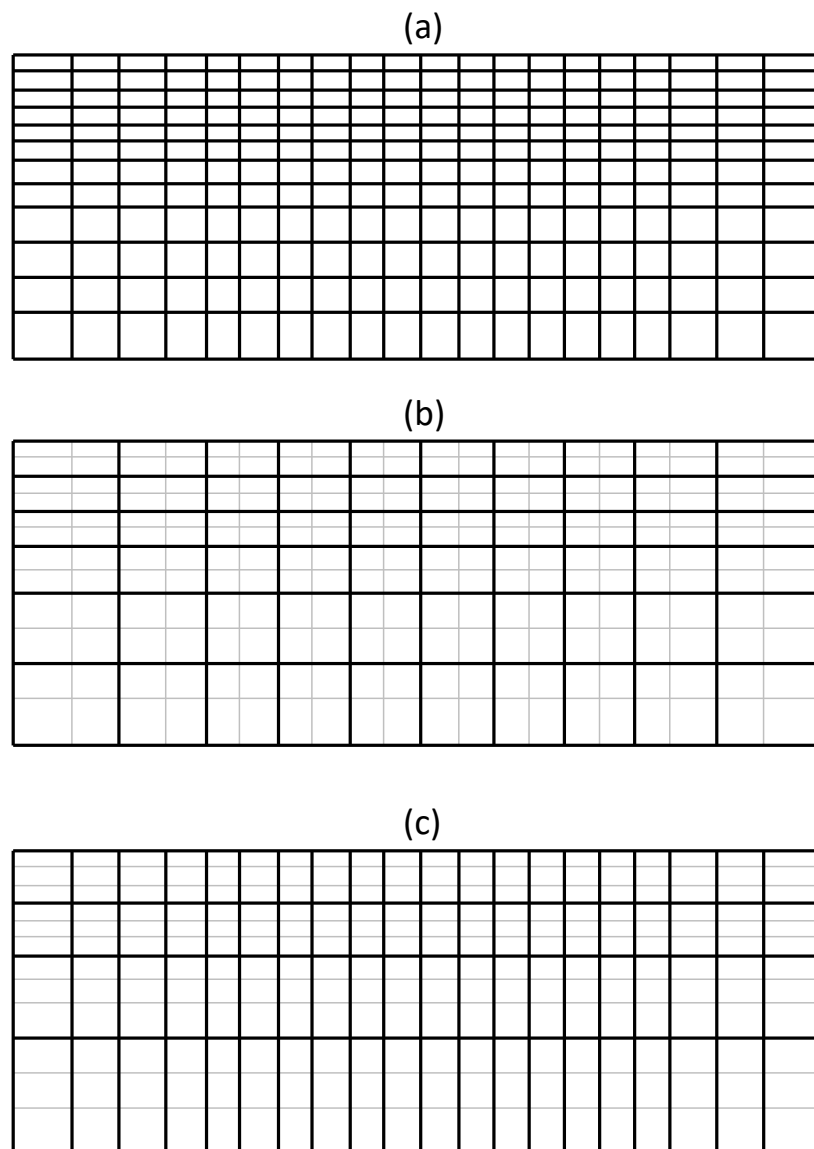


Figure 6.1: Defining parameter boundaries in a structured mesh. The grey lines show the finite element mesh, the black lines show the parameter zones. (a) Each element is a parameter. (b) Each parameter is a 2 x 2 patch of elements. (c) Each parameter is a 3 x 1 patch of elements.

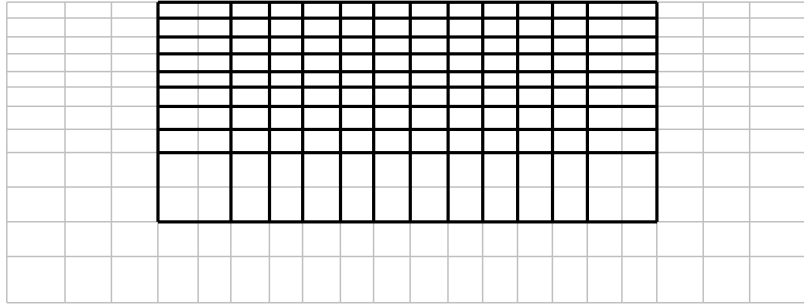


Figure 6.2: Parameterisation of a subset of the structured finite element mesh. The grey lines show the finite element mesh, the black lines show the parameter zones.

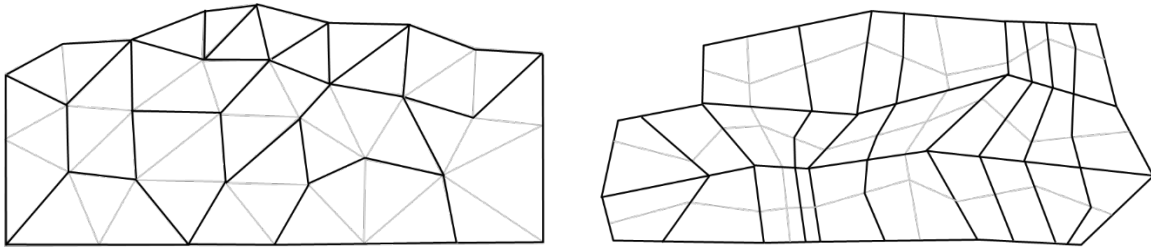


Figure 6.3: Parameterisation of an unstructured mesh defined in **mesh.dat**. The grey lines show the finite element mesh, the black lines show the parameter boundaries.

Further control of parameterisation is achieved through ‘zoning’ of parameters. In **R2** a zone is defined as a congruent collection of parameters (see Figure 6.4). Smoothing (in the inverse solution) does not occur across zones. This can be useful if *a priori* information allows the user to define sharp contrasts (e.g. at a water table boundary).

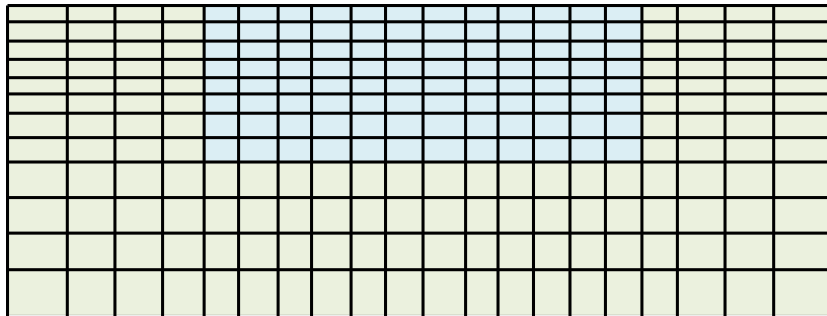


Figure 6.4: Zoning of parameterisation. The two colours represent different parameter zones in the mesh.

Again, full flexibility is possible with an unstructured mesh (see Figure 6.5). For each element the parameter and zone is defined in the **mesh.dat** file.

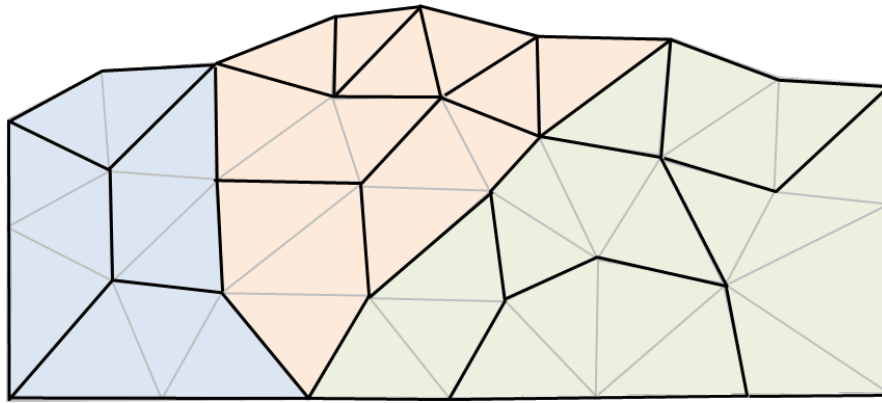


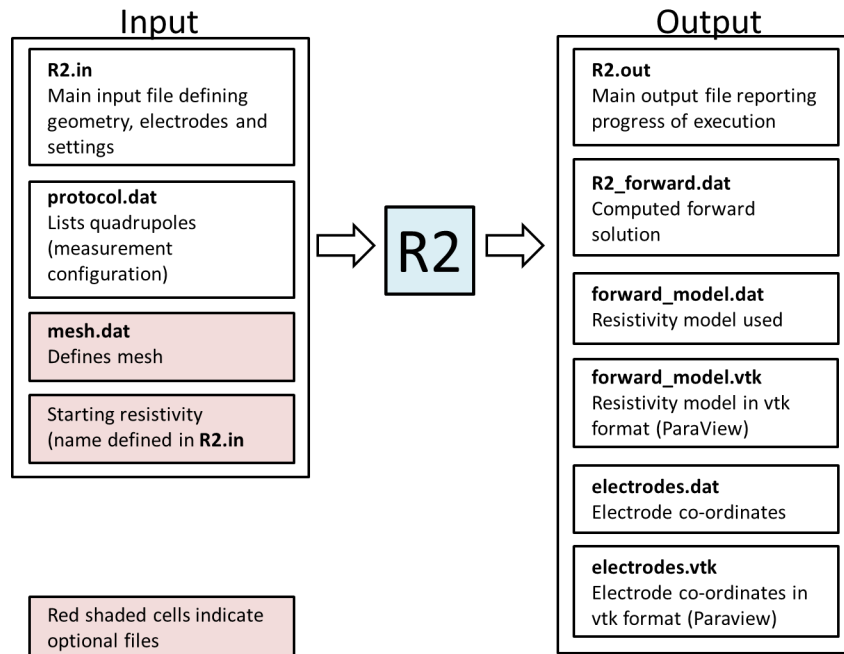
Figure 6.5: Zoning of parameterisation in an unstructured triangular mesh. The three colours represent different parameter zones.

In summary, when a mesh is defined in **mesh.dat**, each element is assigned (i) a parameter number (which is zero if it should remain fixed throughout the inversion); (ii) a zone number. For most cases the parameter number of each element is the element number and the zone is 1.

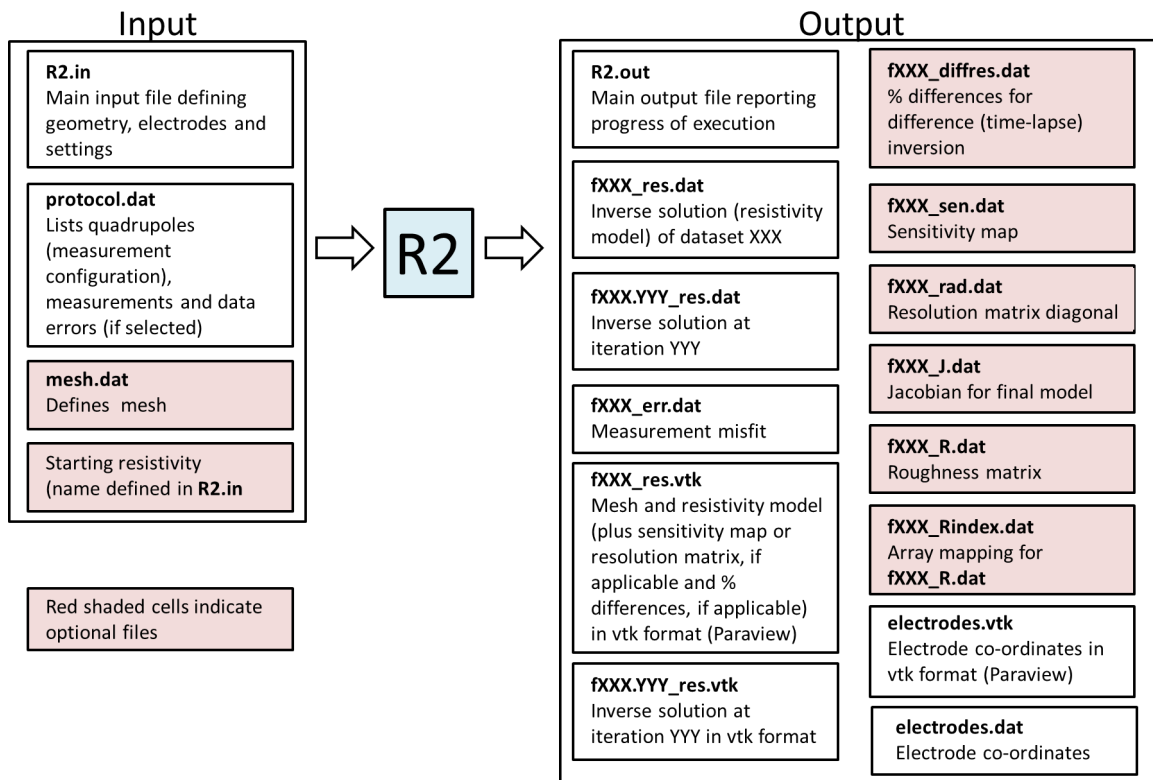
7. Input and output files

The input and output files used by **R2** are shown schematically below, and described in detail later.

Forward mode



Inverse mode



R2 requires at least two input files: **R2.in** and **protocol.dat**. If a pre-defined mesh is used then an additional input file – **mesh.dat** – is required. **R2.in** contains information on the geometry of the problem to be solved. **protocol.dat** contains the four electrode configuration (and measurement for inverse mode). In inverse mode you can repeat datasets in **protocol.dat**.

R2 will output a number of files:

- **R2.out** which will contain main log of execution.
- **electrodes.dat** contains the coordinates of the electrodes.

If the problem to be run is a forward model then **R2** will output:

- **R2_forward.dat** which will contain the forward model for the electrode configuration in **protocol.dat**. The format of **R2_forward.dat** is the same as **protocol.dat** but with 2 extra columns: the first contains the calculated resistances and the second contains the calculated apparent resistivities. Note that the apparent resistivities are computed assuming infinite boundaries and a flat topography at $z=0$. If these do not apply then the computed geometric factors will be incorrect, and consequently the apparent resistivities will be incorrect. If **R2** computes the absolute value of the geometric factor to be less than $1e-10$ then the apparent resistivity that is output is assigned to a value of -100000.00000 in the output file. This does not necessarily mean that the computed transfer resistances are poorly estimated – more likely that the assumptions of infinite boundaries and a flat topography at $z=0$ is not applicable.
- **forward_model.dat** which will contain the resistivity distribution for your forward model (i.e. what you specified in the input for **R2**). Note that the format of these will be the same as described below for inverse mode.
- **forward_model.vtk** as above but vtk format (allowing plotting in **ParaView**, for example).

If the problem to be run is an inverse model then **R2** will output:

- **f001_res.dat** which will contain the resistivity result of the inverse solution. **f001_res.dat** will contain four columns: x , z , $resis$, $\log_{10}(resis)$, where x , z are coordinates at centroid of each element and $resis$ is the resistivity in that element and $\log_{10}(resis)$ is \log_{10} of the resistivity value. The format is setup to work directly with contouring programs like Surfer.
- **f001_err.dat** will contain nine columns. The first four columns contain the electrode numbers. In the fifth column is the normalised data misfit, the next column contains the observed data recorded as an apparent resistivity, the next column contains the equivalent apparent resistivities for the computed model, the next column shows the original data weight (i.e. data standard deviation in same units as data), the next column is the final data weight, the last columns shows a "1" if any weights have been changed during the inversion, otherwise a "0" will appear. **NOTE**: the output format of **f001_err.dat** changed in **R2** v3.2.
- if you select resolution matrix calculation then **f001_rad.dat** will contain the diagonal of the resolution matrix for all elements (see equation 18). A value close to 1 indicates that the parameter for that element can be resolved perfectly, a value close to 0 indicates that the parameter cannot be resolved at all. The format is the same as **f001_res.dat**.
- if you select sensitivity map calculation then **f001_sen.dat** which will contain the diagonal of the matrix $[J^T W^T W J]$ (see equation 20) which gives an idea of the mesh sensitivity coverage. You will get a value for all elements. High values indicate high sensitivity to data, low values indicate poor sensitivity. Plot on a log scale. The format is the same as **f001_res.dat**. In **R2** v4.10 (and subsequent versions) an additional column includes the logarithm of the sensitivity map scaled by the area of the parameter cell (equation 21).

- if you select sensitivity map calculation and output of the Jacobian then three other files will be output: **f001_J.dat** (the Jacobian); **f001_R.dat** (the roughness matrix); **f001_Rindex.dat** (the mapping of the roughness matrix, as the latter is stored in compressed form). All three files will have two integers in line 1. These are the array sizes. Note that the first subscript varies slowest, so if line 1 is “5 10” then an array x of size (5,10) is stored as: $x(1,1)$, $x(1,2)$, ... , $x(1,5)$, $x(2,1)$, $x(2,2)$, ..., $x(5,10)$. The Jacobian is of size number of measurements x number of parameters. The roughness matrix is stored as number of parameters x N, where N will be either 5 or 13 depending on the roughness scheme used. The file **f001_Rindex.dat** shows the mapping of the compressed form of the roughness matrix in **f001_R.dat**, e.g. if line 2 (i.e. the line with the first row of the roughness matrix, given that the first line of the file contains the size of the array) of **f001_Rindex.dat** is “1 2 13 0 0” then in line 2 of **f001_R.dat** the roughness matrix entries $R(1,1)$, $R(1,2)$, $R(1,13)$ are stored. Note that the zeros in **f001_Rindex.dat** mean that no entry exists because this parameter (parameter 1) is only connected to two other parameters (parameters 2 and 13).
- **f001_res.vtk** will contain resistivity, \log_{10} resistivity, \log_{10} sensitivity (if selected) , \log_{10} scaled sensitivity (if selected) and \log_{10} resolution (if selected) in vtk format (allowing plotting in **ParaView**, for example).
- If you have more than one dataset in **protocol.dat** (see later) then the files **f001_res.dat**, **f002_res.dat**, **f003_res.dat**, etc will be created. Similarly, a set of **_err.dat**, **_rad.dat** and/or **_sen.dat** files will be output.
- The output **f001_res.dat** is made at convergence, however, sometimes it is useful to look at the resistivity image at various stages in the iterative process. For all iterations prior to the final iteration a file **f001.XXX_res.dat** will be output, where XXX is 001, 002, 003, etc for the first, second, third, etc iterations. The format of this file is the same as **f001_res.dat**. If multiple datasets appear in **protocol.dat** then corresponding output files will be created. For example, **f003.005_res.dat** will be the fifth iteration of the inversion of the third dataset in **protocol.dat**.
- **f001.XXX_res.vtk** will be output at each iteration and contain the resistivity model in vtk format at iteration XXX (001, 002, etc).
- If a difference inversion is run ($\text{reg_mode} = 2$ in line 21 of **R2.in**) then an additional file will be created for each dataset. **f001_diffres.dat** will contain three columns: x , z , diffres , where x, z are coordinates at centroid of each element and diffres is the percentage change in resistivity from the baseline model. The format is setup to work directly with Surfer.

In addition **R2** will output:

- **electrodes.dat** , which contains the co-ordinates of the electrodes. The values are in three columns: x, z, y (where y is a dummy value – set to 0.0).
- **electrodes.vtk** contains the co-ordinates of the electrodes in vtk format. The values are in three columns: x, z, y (the latter being set to zero). Use this file if you are working with **Paraview** to look at the resistivity images. Once you have opened the electrodes.vtk file in **ParaView** you select “apply” then select “Representation” as “Point Gaussian” and change the radius of the symbols.

NOTE: If **R2** fails to converge in inverse mode, all output files except the sensitivity map/resolution matrix will still be output in order to allow the user to assess the source of the problem (the **fXXX.err** file is useful for this) but the user should check the **R2.out** file to ensure convergence is achieved before using any computed resistivity models.

Some comments on co-ordinate sign convention

When a quadrilateral mesh is created the user specifies the horizontal and vertical co-ordinates of the rows and columns forming the mesh. The convention here (see line 9 in **R2.in**) is for the vertical co-ordinates to be specified as depth (not elevation). When these are output in a **.dat** file (e.g. **forward_model.dat**, for a forward model, or **f001.dat**, for an inversion) then the vertical co-ordinate sign is changed. This is so that programs like Surfer will show the section properly. The same switching of sign is changed in the vtk output (e.g. **forward_model.vtk** and **f001.vtk**). The electrode co-ordinates (output in **electrodes.dat** and **electrodes.vtk**) will also have a switched sign for the vertical co-ordinates.

When defining a mesh in **mesh.dat** meshes should be created with the vertical co-ordinate representing elevation, not depth. And so when such a mesh is used, the sign change is not made in any of the output files listed above.

8. Details of **R2.in**

Line 1: (Char*80) **header**

where **header** is a title of up to 80 characters

Line 2: (2 Int, Real, 2 Int) **job_type**, **mesh_type**, **flux_type**, **singular_type**, **res_matrix**

where **job_type** is 0 for forward solution only or 1 for inverse solution; **mesh_type** is 3 for triangular mesh (see Figure 5.5), 4 for a regular quadrilateral mesh, 5 for a more generalised structured quadrilateral mesh (see Figure 5.3c), 6 for a general quadrilateral mesh (see Figure 5.4); **flux_type** is 2.0 for 2D current flow (i.e. line electrodes, which are infinitely long orthogonal to the section) or 3.0 (usual mode) for fully 3D current flow (i.e. point electrodes); **singular_type** is 1 if singularity removal (see Lowry et al., 1989) is to be applied (otherwise 0). Note that singularity removal can only be applied is (a) the boundaries are infinite and (b) the $z=0$ plane defines the upper boundary; (c) the upper boundary is flat (if any of these conditions do not apply then singularity removal cannot be used); **res_matrix** is 1 if a 'sensitivity' matrix is required for the converged solution. This matrix is not the Jacobian but is the diagonal of $[J^T W^T W J]$ which gives an idea of the mesh sensitivity (see equation 20). One value is stored for each finite element in the mesh. High values indicate high sensitivity, low values indicate poor sensitivity. Plot on a log scale. Set **res_matrix** to 2 if the true resolution matrix is computed for a converged solution and the diagonal is stored (see equation 18), note that this calculation is more time consuming than the 'sensitivity matrix' option. Set **res_matrix** to 3 if the sensitivity map is required and an output of the Jacobian matrix and roughness matrix. If neither sensitivity map or resolution matrix is required then set **res_matrix** to 0

If **mesh_type** is 3 or 6 then the file **mesh.dat** must be supplied which contains the mesh details including node coordinates and element indices (see details later).

If (**mesh_type** = 4) then a regular quadrilateral mesh is to be used and the following are read:

Line 3: (2 Int) **numnp_x**, **numnp_z**

where **numnp_x** is number of nodes in the x direction (horizontal) and **numnp_z** is the number of nodes in the z (vertical) direction

Line 4: (numnp_x Real) **xx**

where **xx** is an array containing x coordinates of each of **numnp_x** node columns

Line 5: (numnp_x Real) **topog**

where **topog** is an array containing elevations of each of **numnp_x** node columns. If the topography is flat then set **topog** to zero for all values.

Line 6: (numnp_y Real) **zz**

where **zz** is an array containing the depths of each of **numnp_z** node rows relative to the **topog array**. Set **zz(1)** to zero and the other values to a positive number (i.e. **zz** represents depth, not topography).

Else if (**mesh_type** = 5) then a more generalised structured quadrilateral mesh is to be used and the following are read:

Line 7: (2 Int) **numnp_x**, **numnp_z**

where `numnp_x` is number of nodes in the x direction (horizontal) and `numnp_z` is the number of nodes in the z (vertical) direction

Line 8: (numnp_x Real) `xx`

where `xx` is an array containing x co-ordinates of each of `numnp_x` node columns

Line 9: (numnp_y Real) `zz`

where `zz` is an array containing elevations (not depths) of each of `numnp_z` node rows for column 1 in the x direction. For each column of nodes `zz(1)` is the topography.

Repeat Line 9 for all `numnp_x` columns.

End if

Note: It is wise to add a carriage returns to break up a long list of input values (in Line 4, 5, 6, 8 and 9, for example). Don't write more than 20 numbers on each line as the compiler may not like it.

If (`mesh_type = 3`) then read the following

Line 10: (Real) `scale`

where `scale` is a scaling factor for the mesh co-ordinates. This is usually 1.0 but if a standardised mesh is used, say for a unit circle, then this scaling factor is useful to adjust the mesh for a specific problem. Set `scale=1` if you do not wish to change the coordinates of the mesh defined in **mesh.dat**.

End if

Line 11: (Int) `num_regions`

where `num_regions` is number of resistivity regions that will be specified either as starting condition for inverse solution or actual model for forward solution. The term "region" has no significance in the inversion – it is just a means of inputting a non-uniform resistivity as a starting model for inversion or for forward calculation.

If (`num_regions = 0`) then read the following

Line 12: (15*Char) `file_name`

where `file_name` is the name of the file containing the resistivities from a previous inversion (the **_res.dat** file that had been produced). Note that the `file_name` must be no more than 15 characters and there should be no spaces before the file name and no characters in the line after the file name.

Else

Line 13: (2 Int, Real) `elem_1, elem_2, value`

where the resistivity `value` will be assigned for all elements from `elem_1` to `elem_2` (inclusive). Note that for a quadrilateral mesh the elements are numbered down columns first (top to bottom) then along rows (left to right).

Repeat Line 13 for all `num_regions`

End if

NOTE: you must assign all elements a starting value. The number of elements in the mesh is $(numnp_x-1) \times (numnp_y-1)$ for a structured quadrilateral mesh. All these elements must be assigned a resistivity. Note also that if you assign an element a value, it will overwrite any previous assignment.

If (`job_type = 1`. i.e. an inverse solution) then read the following

If (`mesh_type = 4` or `5`) then read the following

Line 14: (2 Int) `patch_size_x, patch_size_z`

where `patch_size_x` and `patch_size_z` are the parameter block sizes in the x and z direction, respectively. We differentiate between parameter size and element size to allow faster computation. The larger the patch size the few parameters and the faster the inversion, however, if we increase it too much we will reduce the flexibility to create variation of resistivity. If computational time is not a problem then use a patch size of 1 for x and z. Note that the number of elements in the x direction must be perfectly divisible by `patch_size_x` and the number of elements in the z direction must be perfectly divisible by `patch_size_z` otherwise set them both to zero. See examples in Figure 6.1. For Figure 6.1a `patch_size_x = 1` and `patch_size_z = 1`. For Figure 6.1b `patch_size_x = 2` and `patch_size_z = 2`. For Figure 6.1c `patch_size_x = 1` and `patch_size_z = 3`.

If (`patch_size_x = 0`) and (`patch_size_z = 0`) then read the following

Line 15: (2 Int) `num_param_x, num_param_z`

where `num_param_x` and `num_param_z` are the number of parameter blocks in the x and z directions

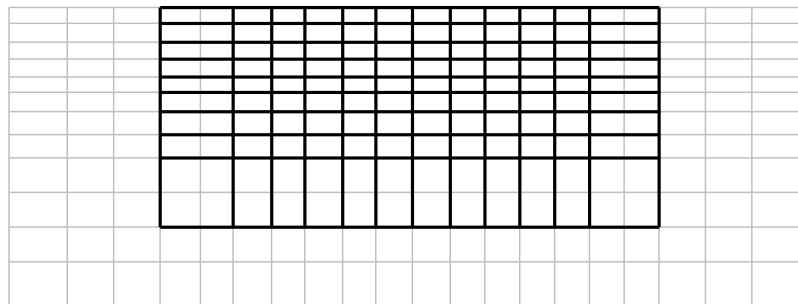
Line 16: (1+`num_param_x` Int) `npxstart, npx(i), i=1,num_param_x`

where `npxstart` is the column number in the mesh where the parameters start; `npx` specifies the number of elements in each parameter block in the x direction

Line 17: (1+`num_param_y` Int) `npzstart, npz(i), i=1,num_param_z`

where `npzstart` is the row number in the mesh where the parameters start; `npz` specifies the number of elements in each parameter block in the z direction

See example in Figure 6.2 (copied below). For this example we would set `num_param_x = 12` and `num_param_z = 9`. Then we would set Line 16 as 3, 2,1,1,1,1,1,1,1,1,2 and Line 17 as 1, 1,1,1,1,1,1,1,2.



End if

End if

NOTE: the following line input is different to v2.7c and older versions of R2

Line 18: (Int, Real) `inverse_type`, `target_decrease`

where `inverse_type` is 0 for pseudo-Marquardt solution or 1 for regularised solution with linear filter (usual mode) or 2 for regularised type with quadratic filter or 3 for qualitative solution or 4 for blocked linear regularised type (see also line 24). Note that the blocking defined here is only for a quadrilateral mesh – for blocking within a triangular mesh see the details for preparing **mesh.dat** later. `target_decrease` is a real number which allows the user to specify the relative reduction of misfit in each iteration. A value of 0.25 will mean that **R2** will aim to drop the misfit by 25% (and no more) of the value at the start of the iteration. This allows a slower progression of the inversion, which can often result in a better convergence. If you set `target_decrease` to 0.0 then **R2** will try to achieve the maximum reduction in misfit in the iteration.

if (`inverse_type` = 3) then

Line 19: (Int) `qual_ratio`

where `qual_ratio` is 0 for qualitative comparison with forward solution, i.e. only when one observed data set is available, or `qual_ratio` is 1 if the observed data in **protocol.dat** contains a ratio of two datasets. This option is a legacy feature of **R2** and is not normally adopted.

Line 20: (2 Real) `rho_min`, `rho_max`

where `rho_min` and `rho_max` are the minimum and maximum observed apparent resistivity to be used. `rho_min` can be negative. Note that if you are computing on an enclosed region (i.e. not an infinite half space), or if the topography is not flat and set to zero, then the apparent resistivities will not be valid and so extreme values should be used in Line 20, e.g. -1.0e10, 1.0e10

Else

NOTE: the following line input is different to v2.4 and older versions of R2

Line 21: (2 Int) `data_type`, `reg_mode`

where `data_type` is 0 for true data based inversion or 1 for log data based. Note that the latter should improve convergence but may not work for internal electrodes (e.g. borehole type) where the polarity can change due to resistivity distributions; `reg_mode` is 0 for normal regularisation; or 1 if you want to include a *background regularisation* relative to your starting resistivity (this is whatever you have set in input lines 11 to 13); or 2 if you wish to regularise relative to a previous dataset using the *difference inversion* of LaBrecque and Yang (2001). If you select `reg_mode`=1 then Line 22 will require a regularisation parameter `alpha_s`. If you select `reg_mode`=2 then **protocol.dat** must contain an extra column (see below) with the reference dataset. In addition, your starting model (see Line 12) should be the inverse model for this reference dataset (i.e. you need to invert the reference dataset before running the time-lapse inversion). Also note that if you select `reg_mode`=2 then `data_type` is automatically set to 0 irrespective of what was entered in Line 21.

NOTE: the following line input is different to v2.4 and older versions of R2

if ((reg_mode = 0) or (reg_mode = 2)) then

Line 22: (Real, 2 Int, Real) tolerance, max_iterations, error_mod, alpha_aniso

Else

Line 22: (Real, 2 Int, 2 Real) tolerance, max_iterations, error_mod, alpha_aniso,
alpha_s

End if

where **tolerance** is desired misfit (usually 1.0); **max_iterations** is the maximum number of iterations; **error_mod** is 0 if you wish to preserve the data weights, 2 if you wish the inversion to update the weights as the inversion progresses based on how good a fit each data point makes. **error_mod=2** is recommended – this is a routine based on Morelli and LaBrecque (1996). Note that no weights will be increased. The smoothing factor used in the code (alpha) is searched for at each iteration. The search is done over a range of steps in alpha, the number of steps is 10. **alpha_aniso** is the anisotropy of the smoothing factor, set **alpha_aniso** > 1 for smoother horizontal models, **alpha_aniso** < 1 for smoother vertical models, or **alpha_aniso=1** for normal (isotropic) regularisation. **alpha_s** is the regularisation to the starting model (if you set **reg_mode** = 1 in Line 21). Set **alpha_s** to a high value (e.g. 10) to highly penalise any departure from this starting model. Note that **alpha_s** will stay fixed – if you set it too high then **R2** may not converge. **R2.out** will report the value of alpha used to regularise smoothing within the image – the regularisation relative to a reference model is additional to this. The user may find setting **alpha_s** useful as a comparison of inversions from two runs with difference reference models allows an assessment of the depth of investigation following the approach of Oldenburg and Li (1999).

Line 23: (4 Real) a_wgt, b_wgt, rho_min, rho_max

where **a_wgt** and **b_wgt** are error model parameters describing the standard deviation of measurements following:

$$\text{std}(R) = \sqrt{(\text{a_wgt} * \text{a_wgt}) + (\text{b_wgt} * \text{b_wgt}) * (R * R)}$$

where R is the resistance measured (LaBrecque et al., 1996 equation 14). Note that it is the inverse of the standard deviation that is used as weight in the diagonal of the weight matrix **W**.

It is advisable to estimate **a_wgt** and **b_wgt** from error checks in the field data (ideally from reciprocal measurements - not measures of repeatability). Typically for surface data **a_wgt** will be about 0.01 Ohms and **b_wgt** will be about 0.02 (roughly equivalent to 2% error). Note that if you select **data_type=1** in Line 21 then although the resistance data are transformed into log apparent conductivities the **a_wgt** and **b_wgt** parameters should still reflect the variance of the resistance; **rho_min** and **rho_max** are the minimum and maximum observed apparent resistivity to be used for inversion (use large extremes if you want all data to be used). If data are ignored by **R2** because of the apparent resistivity limits then these will be reported individually in **R2.out**. **NOTE: that the apparent resistivity calculations assume that you have set the ground surface to z=0 and that the ground surface is flat.** Note also that you can select to include individual errors for each measurement in the data input file **protocol.dat** – to do this **a_wgt** and **b_wgt** should be set to 0.0 – **protocol.dat** will then require an additional column (see later).

Line 24: (num_param_x Int) param_symbol

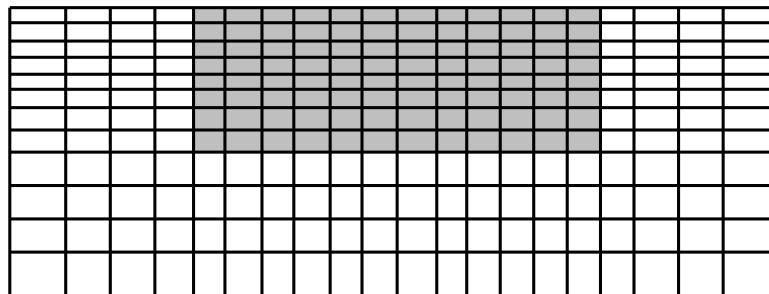
If you have specified zoning of parameters (`inverse_type = 4` in line 18) so that each zone is disconnected from other zones then for a structured quadrilateral mesh (see Figure 6.4) the zones are specified by producing a simple plan of the parameter mesh. You must input for each row of parameters an integer representing the parameters. This is repeated for each row. Make sure that you put a space between each integer. As an example consider the zoned mesh in Figure 6.4 (copied below) with 20 elements in the x direction and 12 elements in the z direction. In this example we wish to zone the region shaded. As each element is a parameter then the patch size in x and z is 1, so in total there are 20 parameters (x) by 12 parameters (z). If we want to set the boundary of the shaded region so that there is no smoothing to the unshaded region then we would input:

```

1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1
1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1
1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1
1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1
1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1
1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1
1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1
1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1
1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

```

Note that we have used 1s and 2s to define the regions. We could have used any other integer.



If for the problem above we had a patch size of 2 in x and z then Line 24 would be:

```

1 1 2 2 2 2 2 2 1 1
1 1 2 2 2 2 2 2 1 1
1 1 2 2 2 2 2 2 1 1
1 1 2 2 2 2 2 2 1 1
1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1

```

If we had defined the problem to have a patch size in x of 4 and a patch size in z of 2 then Line 24 would be:

```

1 2 2 2 1
1 2 2 2 1
1 2 2 2 1
1 2 2 2 1
1 1 1 1 1
1 1 1 1 1

```

Repeat line 24 for all `num_param_z`

End if

End if

NOTE: Lines 25 to 26 define the region to be output (note that this was new to version 2.7)

Line 25: (Integer) `num_xz_poly`

where `num_xz_poly` is the number of x,z co-ordinates that define a polyline bounding the output volume. If `num_xz_poly` is set to zero then no bounding is done in the x-z plane. The co-ordinates of the bounding polyline follow in the next line. **NOTE: the first and last pair of co-ordinates must be identical** (to complete the polyline). So, for example, if you define a bounding square in x,y then you must have 5 co-ordinates on the polyline. The polyline must be defined as a series of co-ordinates in sequence, although the order can be clockwise or anti-clockwise (see examples later). **NOTE: R2 stores the vertical co-ordinates for nodes in a structured quadrilateral mesh with a convention positive upwards. For example, if the ground surface has an elevation of 0m and you wish to output to a depth of 8m then z=-8m must be used for the lower boundary of the polygon. Similarly, if the ground surface elevation is 100m and you wish to output to a depth of 8m then z=-92m must be used for the lower boundary of the polygon. This was not the convention for v2.7a and so any input files created for that version must be changed (this only applies to line 26). If a triangular mesh or quadrilateral mesh in `mesh.dat` is used then the co-ordinates specified in the mesh file are used and the above comments about sign convention do not apply.**

Line 26: (2 Real) `x_poly(1), z_poly(2)`

where `x_poly(1), z_poly(1)` are the co-ordinates of the first point on the polyline.
Repeat line 26 for all `num_xz_poly` co-ordinates.

Line 27: (Int) `num_electrodes`

where `num_electrodes` is number of electrodes

If (`mesh_type` = 3 or 6) then

Line 28: (2 Int) `j, node`

where `j` is the electrode number and `node` is the node number in the finite element mesh

Else

Line 29: (3 Int) `j, column, row`

where `j` is the electrode number, `column` is the column index for the node the finite element mesh and `row` is the row index for the node in the finite element mesh. The `column` value must be in the range 1 to `numnp_x` and the `row` value must be in the range 1 to `numnp_y`. Both values must be integer values.

End If

Repeat Line 29 for all `num_electrodes`

END OF INPUT FOR **R2.in**

9. Details of **protocol.dat**

protocol.dat contains measurement schedule (and data for inverse if selected)

Line 1: (Int) `num_ind_meas`

where `num_ind_meas` is number of measurements to follow in file

If (`job_type = 1`) then

Line 2: (5 Int, 3 Real) `j`, `elec(1,k)`, `elec(2,k)`, `elec(3,k)`, `elec(4,k)`, `v_i_ratio`, `v_i_ratio_0`, `data_sd`

where `j` is not used (but usually is used as a measurement number); `elec(1,k)` is the electrode number for the (M) P+ electrode; `elec(2,k)` is the electrode number for the (N) P- electrode; `elec(3,k)` is the electrode number for the A (C+) electrode; `elec(4,k)` is the electrode number for the B (C-) electrode; `v_i_ratio` is measured resistance value (or ratio of two measured values if `inverse_type=2` and `qual_ratio=1` in **R2.in**); `v_i_ratio_0` is the resistance data for background case (only read if `reg_mode=2`); `data_sd` is data standard deviation (must be positive and only read if `a_wgt` and `b_wgt` in line 23 of **R2.in** are both zero). **NOTE: `v_i_ratio` should contain the polarity of the measurement – do not assign only absolute values.**

Repeat Line 2 for all `num_ind_meas`

Else

Line 3: (5 Int) `j`, `elec(1,k)`, `elec(2,k)`, `elec(3,k)`, `elec(4,k)`

where `j` is not used (but usually is used as a measurement number); `elec(1,k)` is the electrode number for the M (P+) electrode; `elec(2,k)` is the electrode number for the N (P-) electrode; `elec(3,k)` is the electrode number for the A (C+) electrode; `elec(4,k)` is the electrode number for the B (C-) electrode

Repeat Line 3 for all `num_ind_meas`

End if

You can add as many datasets to the file **protocol.dat**. Just concatenate the datasets into one file. **R2** will continue to read and process data using the settings defined in **R2.in**

END OF INPUT FOR **protocol.dat**

10. Details of **mesh.dat**

It is useful if your mesh generator permits 'materials' to be defined, allowing some zoning of the mesh (to permit blocking at interfaces). Also, you may find it beneficial (for computational efficiency) to create a coarse mesh to define the parameters and then refine this mesh (splitting a triangle element into more elements) to have more elements for the forward solution. The simplest mesh consists of an equal number of parameters and elements and one zone. More complex arrangements allow for grouping of elements into parameters and multiple zones. Regularisation is not applied at the interface of zones.

NOTE: Line 1 changed from version 3.3

Line 1: (3 Int) **numel**, **numnp**, **ndirichlet**

Where **numel** is the number of triangle elements, **numnp** is the number of nodes and **ndirichlet** is the node number of a specified dirichlet node, which should be a node far away from all electrode nodes. If **ndirichlet** is set to zero then the code will compute the node that is furthest away. However, for some geometries (e.g. a circular region) the node that is the furthest away based on average distance may be close to one of the nodes. For such problems it is advisable to set the node in the centre of the mesh as the dirichlet node to avoid biasing of the computed potential field.

Line 2: (6 Int) **n**, **index(1,n)**, **index(2,n)**, **index(3,n)**, **param(n)**, **zone(n)**

Where **n** is the element number; **index(1,n)**, **index(2,n)** and **index(3,n)** are the node numbers of the element, numbered in a **counter-clockwise direction** (**R2** will check if this is correct for a triangular or quadrilateral mesh that is read from **mesh.dat**); **param(n)** is the parameter number of the element (to make every element a parameter then make this value equal to the element number); **zone(n)** is the zone number for element **n**. To have one zone make **zone(n)** equal to 1 for all elements. Zones must be connected elements. Parameters cannot occupy more than one zone. **NOTE** also, to make an parameter fixed to the starting resistivity, set **param(n)** to zero but note that if this is done all elements with **param(n) = 0** must be at the end of the block of elements (see Surface 8 example below). This will involve reordering elements and care must be taken to ensure that any associated files with the element mapping (e.g. a start resistivity file, if used) but follow the same new element numbering. Note that **param(n)** and **zone(n)** are not used in forward mode but these columns still need to be added to **mesh.dat**

Repeat line 2 for all **numel** elements.

Line 3: (Int, 2 Real) **n**, **x(n)**, **z(n)**

Where **n** is the node number; **x(n)**, **z(n)** are the coordinates of node **n**.

Repeat line 3 for all **numnp** nodes.

END OF INPUT FOR **mesh.dat**

11. Examples

The folder “Examples” contains a number of worked examples of **R2** to illustrate how to setup input files and work with model output.

11.1 Surface electrode array 1 – getting started

The subfolder “Examples/Surface_1/dpdp” contains an example synthetic model of a surface electrode array using a dipole-dipole measurement scheme. The example is taken from Binley and Kemna (2005). For this problem 25 electrodes are positioned at 2m spacing on a flat surface of a half space. The electrodes are numbered 1 to 25 from left to right. A forward model is setup to determine the measured transfer resistances for a dipole-dipole scheme with 117 measurements. The resistivity model is shown in Figure 11.1. A small target with resistivity $10 \Omega\text{m}$ lies within a $100 \Omega\text{m}$ half space: positioned vertically between depths 1m and 4m and horizontally between 14m and 16m.

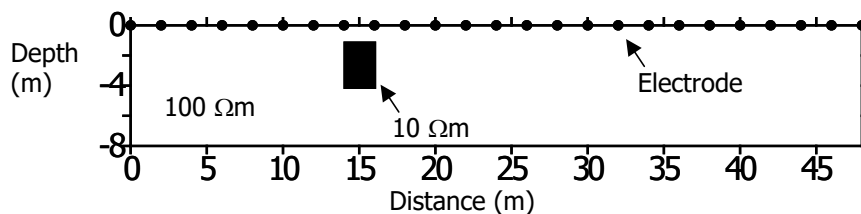


Figure 11.1: Definition of synthetic model for surface array 1 problem

The subfolder “Examples/Surface_1/dpdp/Forward” contains the **protocol.dat** file for the forward problem. Also contained in the folder is the file **R2.in** which defines the geometry and resistivity model. Since the model is a half space the finite element mesh must extend significantly away from the region of investigation (horizontally and vertically downwards). The mesh developed consists of 225 node columns and 49 node rows (i.e. 11,025 nodes, 10,752 elements). The file **R2.in** shows how the mesh is designed to get progressively coarser away from the region of study. Note that the co-ordinates of the mesh have been set so that electrode 1 is at (0,0) for this problem. In the mesh electrode 1 is located at node column 17 (i.e. there are 16 elements to the left of the electrode array to represent an infinite boundary condition to the left. For this example 8 elements are placed between electrodes and so node 2 is at node column 25, node 3 is at column 33, etc. Since the electrodes are located on the ground surface the row node for all electrodes is 1. All the electrode positions are assigned in **R2.in**. The file also assigns the resistivity for all elements. For this problem it is done by defining the resistivity of 9 congruent blocks of elements. First all elements in the mesh are set to $100 \Omega\text{m}$ and then 8 columns of vertically adjacent elements are defined to set the $10 \Omega\text{m}$ anomaly (remember that the elements are numbered vertically then horizontally).

When **R2** is run the output files are:

R2.out, which contains the main log of execution

electrodes.dat, which contains the electrode co-ordinates

R2_forward.dat, which contains the forward model, i.e. the 117 transfer resistances. Note that the apparent resistivity for each of the 117 measurements is also stored.

forward_model.dat, which contains the co-ordinates of the centroid of each finite element in the mesh, the resistivity of each finite element along with the logarithm (to base 10) of the resistivity. This file is useful for checking if the resistivities were defined correctly in **R2.in**

In Binley and Kemna (2005) the same forward model is presented in pseudo section format.

The subfolder “Surface_1/dpdp/Inverse” contains files for running the inversion of the transfer resistances determined above. For this a uniform starting resistivity of $100 \Omega\text{m}$ is defined in the file **R2.in**. The ‘data’ to be inverted is stored in file protocol.dat: here the values are simply the transfer resistances that appeared in the **R2_forward.dat** file described earlier.

For the inverse problem we have used a `patch_size` of 4 in both x and z directions, i.e. each inverse parameter is a 4 by 4 block of finite elements.

When **R2** is run in this case the output files are:

- R2.out**, which contains the main log of execution;
- electrodes.dat**, which contains the electrode co-ordinates;
- f001_res.dat**, which contains the computed resistivity (and \log_{10} resistivity) for each finite element (in the entire mesh – not just the region of interest);
- f001_err.dat**, which contains the misfit for each of the 117 measurements;
- f001_sen.dat**, which contains the sensitivity map computed using equation 20;
- f001.001_res.dat**, which contains the computed resistivity (and \log_{10} resistivity) for each finite element after the first iteration. Note that the inversion converged after 2 iterations for this problem and so this is the only intermediate solution.

Figure 11.2 shows the results of the inversion (compare with Fig 5.8 of Binley and Kemna(2005)). This is an image map of the results in `f001_res.dat` (x and y in columns 1 and 2 and logarithm of resistivity in column 4). Note that only the region within the electrode array and to a depth of 8m has been plotted.

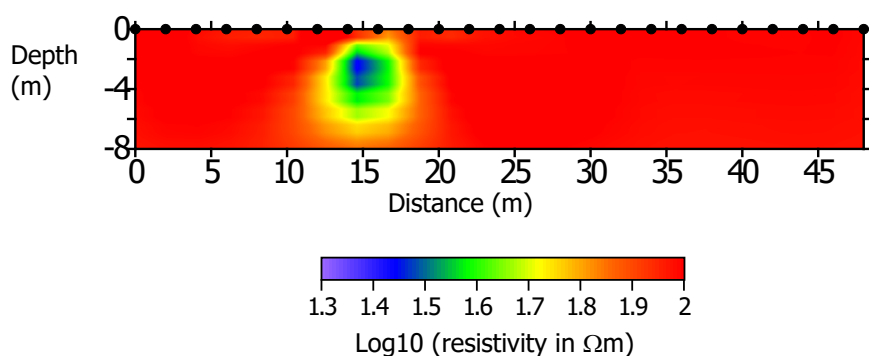


Figure 11.2: Inverse model for surface array 1 problem with dp-dp array

In Figure 11.3a the sensitivity map is shown (`res_matrix` in line 2 of **R2.in** is set to 1). The values are computed with equation 20. High values indicate areas of high measurement sensitivity. It is often useful to use this map to mask the resistivity image (see example on cover page of this document). Showing values of the sensitivity map < 0.001 of the maximum value as opaque is a useful guide for this. Figure 11.3b shows the sensitivity map with each value scaled by the parameter cell area. In this case the overall pattern is no different to the unscaled version since the finite element mesh is uniformly discretised. However, for meshes where there is considerable variation in element sizes (and hence parameter cell sizes) then the scaled version of the sensitivity map is likely to be more useful.

Had the problem been run with `res_matrix` in line 2 of **R2.in** set to 2 then the diagonal of the resolution matrix would have been computed. This is useful for comparing models and measurement schemes. In Figure 11.4 the map of the resolution matrix diagonal is shown. Values should be ideally equal to 1 (logarithm equal to 0) – values less than this indicate the effect of smoothing on the parameter value (influence of adjacent parameter values). The map of the diagonal of the resolution matrix is very useful for determining a suitable filter for displaying results.

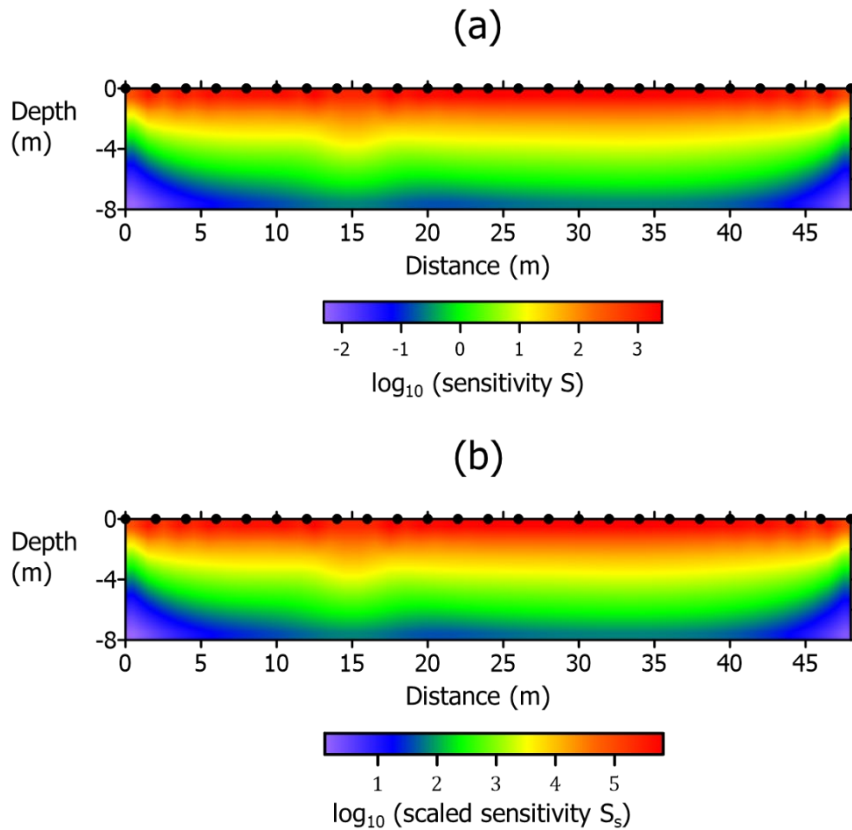


Figure 11.3: Sensitivity map for inverse model for surface array 1 problem with dp-dp array. (a) image is unscaled; (b) image is scaled by parameter cell area.

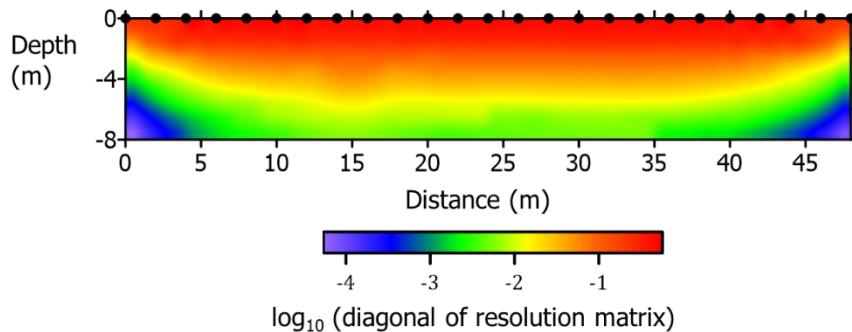


Figure 11.4: Diagonal of resolution matrix for inverse model for surface array 1 problem with dp-dp array

The subfolder "Surface_1/Wenner/Forward" contains files for running a forward model for the same problem but using a Wenner configuration (see figure 5.7 of Binley and Kemna(2005) for the pseudo section. The subfolder "Surface_1/Wenner/Inverse" contains the files for running the inverse model. Figure 11.5 shows the resulting model. Figure 11.6a shows the sensitivity map for this problem; Figure 11.5b shows the diagonal of the resolution matrix for this solution, both illustrating a weaker resolution in comparison to the dipole-dipole array (c.f. Figure 11.3 and 11.4).

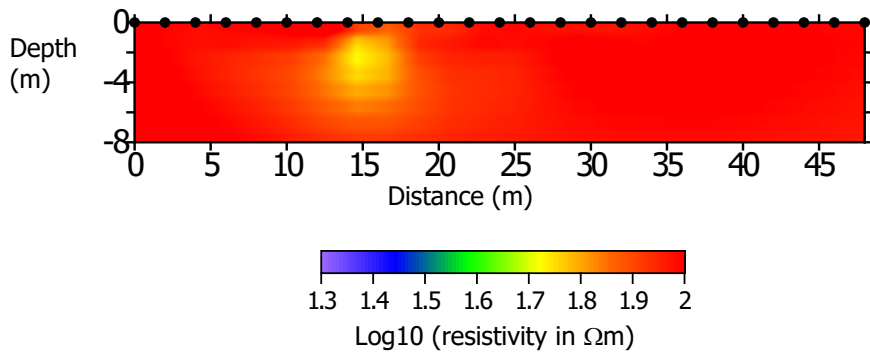
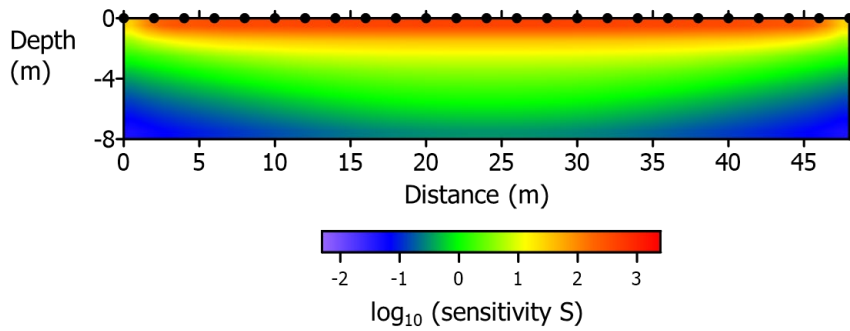


Figure 11.5: Inverse model for surface array 1 problem with Wenner array

(a)



(b)

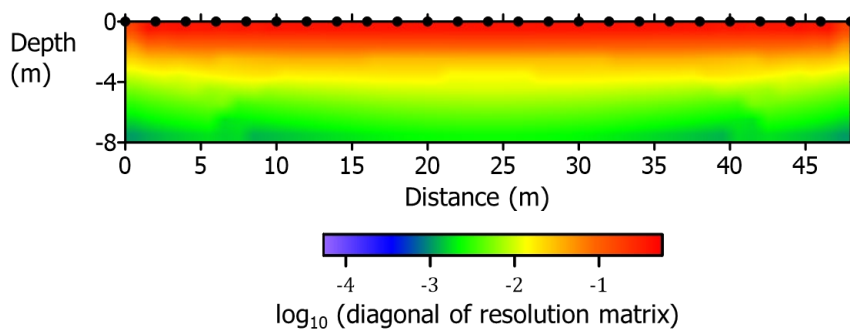


Figure 11.6: Model appraisal for surface array 1 problem with Wenner array. (a) Sensitivity map; (b) diagonal of resolution matrix. The colour scales used are identical to the equivalents for the dp-dp array (Figure 11.3a and Figure 11.4).

11.2 Surface electrode array 2 – adding topography

The subfolder “Examples/Surface_2/dpdp” contains an example similar to the previous case but with varying surface topography. Here the ground surface slopes from 0m at electrode 1 to 4.8m at electrode 25 (see Figure 11.7). The file **R2.in** is now different for the forward and inverse model runs through the addition of topography data. Figure 11.8 shows the inverse solution for this case.

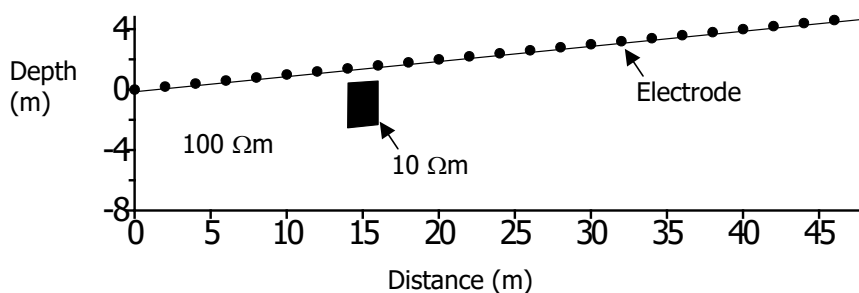


Figure 11.7: Definition of synthetic model for surface array 2 problem

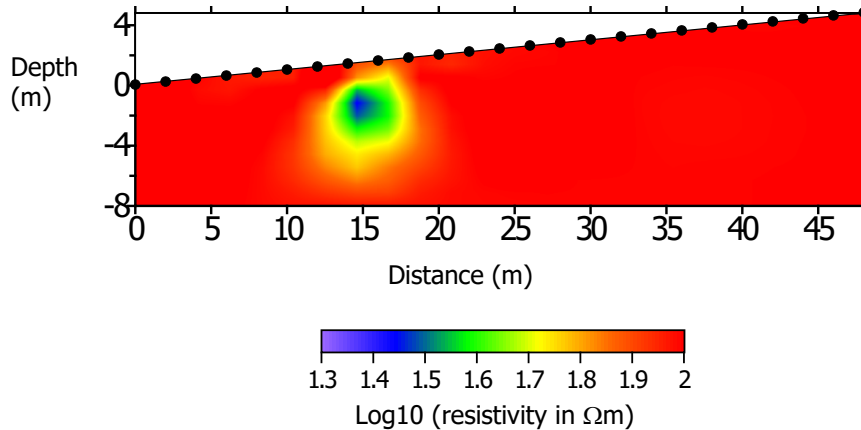


Figure 11.8: Inverse model for surface array 2 problem with dipole-dipole array

11.3 Surface electrode array 3 – fixing parameter values

Occasionally it is useful to fix resistivity values within the mesh. This is particularly useful for time lapse imaging where we wish to focus on changes within a particular part of the mesh. In **R2** this can be achieved with a quadrilateral mesh by defining left, right, upper and lower limits of the parameter zone (see Line 16 and line 17 definitions for **R2.in**). To illustrate this we invert data from a previous example but constrain the parameter zone to a smaller region of the mesh.

The subfolder “Examples/Surface_3/dpdp” contains an example similar to the Surface array 1 example but this time the inverse model is defined so that not all elements are parameters. The forward model used for generating the data file (protocol.dat) is that from Figure 11.1, i.e. in “Examples/Surface_1/dpdp/Forward”.

For this example we use a patch_size of zero in the x and z directions and then define the location of the zone to be parameterised. In **R2.in** a patch of 4 elements per parameter is defined in the horizontal direction starting at element 1. All elements are grouped into parameters in the horizontal and thus there are 56 patches of 4 elements declared (a total of 224 elements). In the vertical we define the parameter zone to be from 1m to 6m depth and a patch size of 2 elements is used (10 parameters in total corresponding to the 20 elements). The starting element for the parameterisation in the vertical is 5 (since the first four elements cover the first 1m in this case). Note that the resistivity of any element that is not declared to contribute to a parameter remains unchanged from the starting value (in this case 100 Ωm).

Figure 11.9 shows the resultant inverse model. The sharp boundaries (in the vertical) at 1m and 6m are a result of the constrained parameter zone (there is no smoothing over the boundaries).

Note that if you restrict the parameter zone too much then convergence of the solution may be problematic (since you will be reducing the degrees of freedom of the inverse solution).

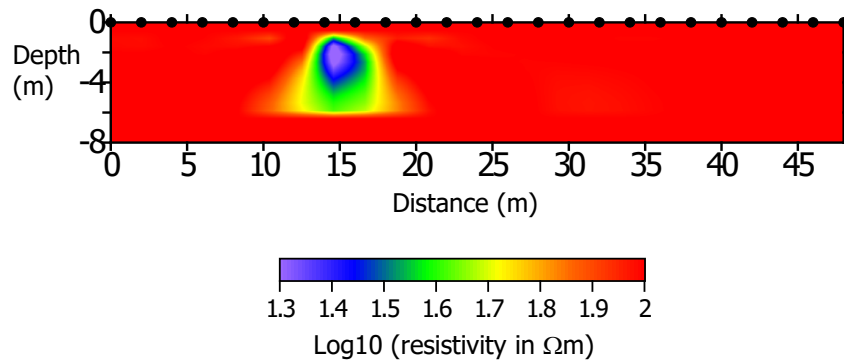


Figure 11.9: Inverse model for surface array 3 problem

11.4 Surface electrode array 4 – anisotropic smoothing

The subfolder “Examples/Surface_4/dpdp” contains an example similar to the Surface array 1 example but this time the smoothing is set to be anisotropic. For this case the smoothing is exaggerated in the vertical by setting `alpha_aniso` in Line 22 of `R2.in` to 0.1 (10 times more smoothing in the vertical). Figure 11.10 shows the resultant inversion (c.f. Figure 2 with isotropic smoothing).

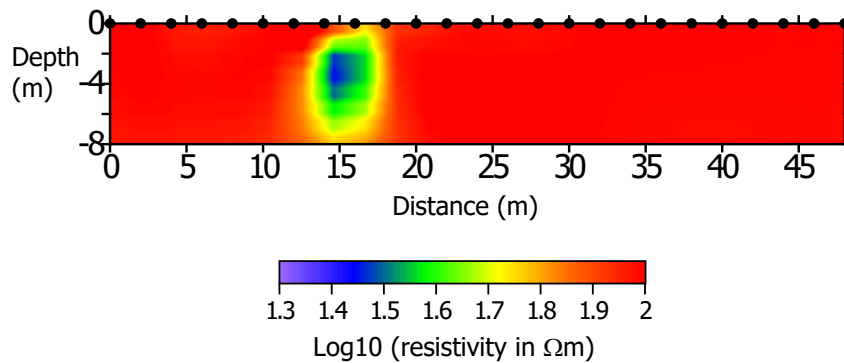


Figure 11.10: Inverse model for surface array 4 problem

11.5 Surface electrode array 5 – more complex meshing

The quadrilateral mesh examples so far have used a simple mesh definition. For the surface array 2 example the mesh was distorted by changing the topography of the upper surface of the mesh. In this example we illustrate how to change the mesh in a more flexible manner. By setting `mesh_type` to 5 in Line 2 of `R2.in` we can specify the row coordinates for every column of the mesh. This requires more input information than the previous examples but gives much greater flexibility.

The subfolder “Examples/Surface_5/dpdp/Forward” contains a forward modelling example similar to the Surface array 1 example but in this case a zone of low resistivity lies just below the ground surface and varies in thickness from 0.5m at electrode 1 to 1m at electrode 25. In addition, the electrodes are located in this example at the bottom of this conductive zone (see Figure 11.11). Such a model may be representative of electrical imaging using electrodes placed at the bed of a stream (the conductive zone representing the stream).

To setup this forward model the 49 row coordinates are defined for all 225 column positions. In addition, `R2.in` must also contain the definition of more groups of elements than before to represent the conductive zone (remember that the zones are defined as groups of congruent elements and since the elements are numbered in the vertical then we must define 224 such groups for this problem, in addition to the rest of the region, i.e. 225 groups in all).

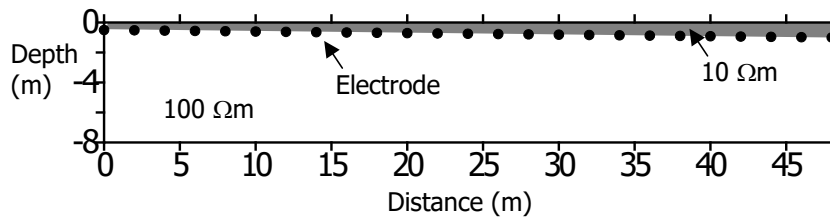


Figure 11.11: Forward model for surface array 5 problem

11.6 Surface electrode array 6 – depth of investigation

The subfolder “Examples/Surface_6” contains three examples illustrating the use of a reference resistivity model. The examples use the dipole-dipole forward model from Surface electrode array 1 but invert three different cases with `reg_mode` set to 1 (see line 21 of **R2.in**).

In case_01 we set α_s to 10 with a resistivity background (starting model or reference model) equal to a uniform $\rho_{\text{back}}=100\Omega\text{m}$. The results are shown in Figure 11.12a. The result is similar to that shown in Figure 11.2 (no regularisation relative to a reference model).

In case_02 we set α_s to 50 with a uniform $\rho_{\text{back}}=100\Omega\text{m}$. The results are shown in Figure 11.12b. The target recovery is now weaker as the inversion applies more penalty to deviation from $100\Omega\text{m}$.

In case_03 we set α_s to 10 with a uniform $\rho_{\text{back}}=50\Omega\text{m}$. The results are shown in Figure 11.12c. Recalling that the background resistivity in the forward model is $100\Omega\text{m}$, Figure 13c illustrates the zone over which the measurements have sensitivity – the lower left and right regions are clearly not influenced by the measurements in this case (which is consistent with the resolution matrix in Figure 11.4).

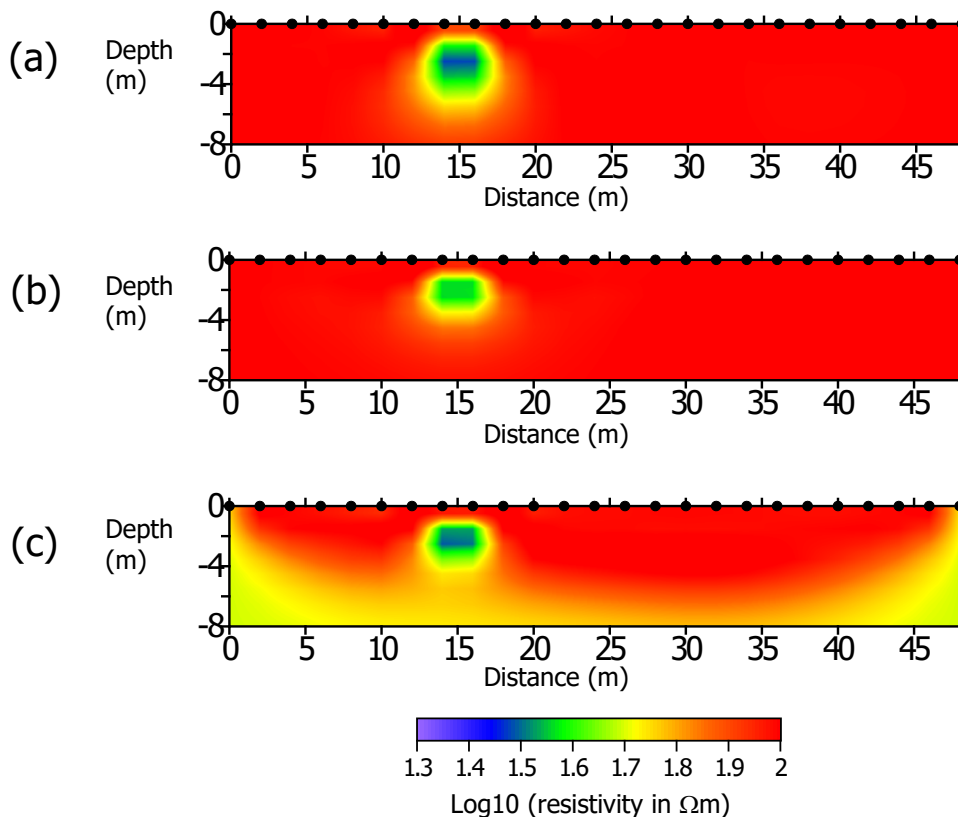


Figure 11.12: Surface array 6 – regularising relative to a reference resistivity model. (a) $\alpha_s=10$, $\rho_{\text{back}}=100\Omega\text{m}$. (b) $\alpha_s=50$, $\rho_{\text{back}}=100\Omega\text{m}$. (c) $\alpha_s=10$, $\rho_{\text{back}}=50\Omega\text{m}$.

We can use these results to assess the depth of investigation (DOI), following the method of Oldenburg and Li (1999). We can compute the value:

$$R(x, y) = \frac{m_1(x, y) - m_2(x, y)}{m_{1,r} - m_{2,r}}$$

Where m_1 are the inversion results in Figure 12a (in log units) using $100\Omega\text{m}$ as a reference and m_2 are the inversion results in Figure 11.12c (in log units) using $50\Omega\text{m}$ then, $m_{1,r} = \log_{10}(100)$ and $m_{2,r} = \log_{10}(50)$. Figure 11.13 shows the variation of R . Oldenburg and Li (1999) suggest a reasonable value of $R = 0.1$ or 0.2 as a suitable depth of investigation. Figure 11.13 shows a contour of $R = 0.2$ to illustrate this.

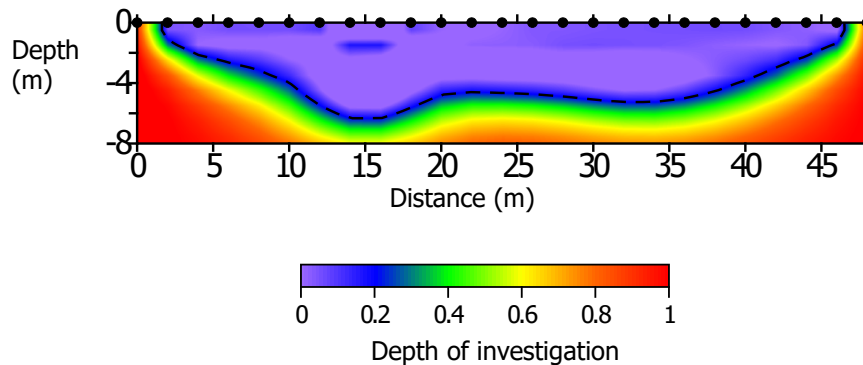


Figure 11.13: Depth of investigation for Surface array 6 problem.

11.7 Surface electrode array 7 – time-lapse (difference) inversion

The subfolder “Examples/Surface_7” contains an example illustrating the use of a difference inversion, which may be useful for time-lapse (monitoring) studies. Here we use two forward models as datasets representing changes in resistivity from time 0 to time 1 (see Figure 11.14).

“Examples\Surface_7\dppd\Forward_t0” contains input files for running a forward model at time 0 and “Examples\Surface_7\dppd\Forward_t1” contains input files for running a forward model at time 1. In each case **R2** produces the file **R2_forward.dat**, which contains the transfer resistances due to the resistivity structure defined. The two **R2_forward.dat** files will be used to create an input data file for a difference inversion.

If we select a difference inversion the data file for inversion (**protocol.dat**) contains two columns of data, as defined earlier in this document. The first column is the measured data (here, at time 1) and the second column is the reference dataset (here, at time 0). The folder “Examples\Surface_7\dppd\Inverse_difference” contains input files for the difference inversion.

For a difference inversion the starting model for the inversion (which is often just a homogenous model for normal inversions) is the resistivity that is consistent with the reference dataset. For this synthetic example we need to determine this model by inverting the forward model at time 0. This is equivalent to Surface electrode array 1, but note that we must save the entire resistivity model, not just the region of interest. **Start_resis.dat** is resulting inversion of the forward model from time 0.

Figure 11.15 shows the results (in **f001_res.vtk**) plotted as log resistivity, using **ParaView**. The electrode locations (from file **electrodes.vtk**) are also shown.

When running a difference inversion an output file **f001_diffres.dat** is produced (in addition to the normal inverse output files). **f001_diffres.dat** provides values of percentage change (from the starting model) in resistivity. The file **f001_res.vtk** also contains this information and is illustrated in Figure 11.16.

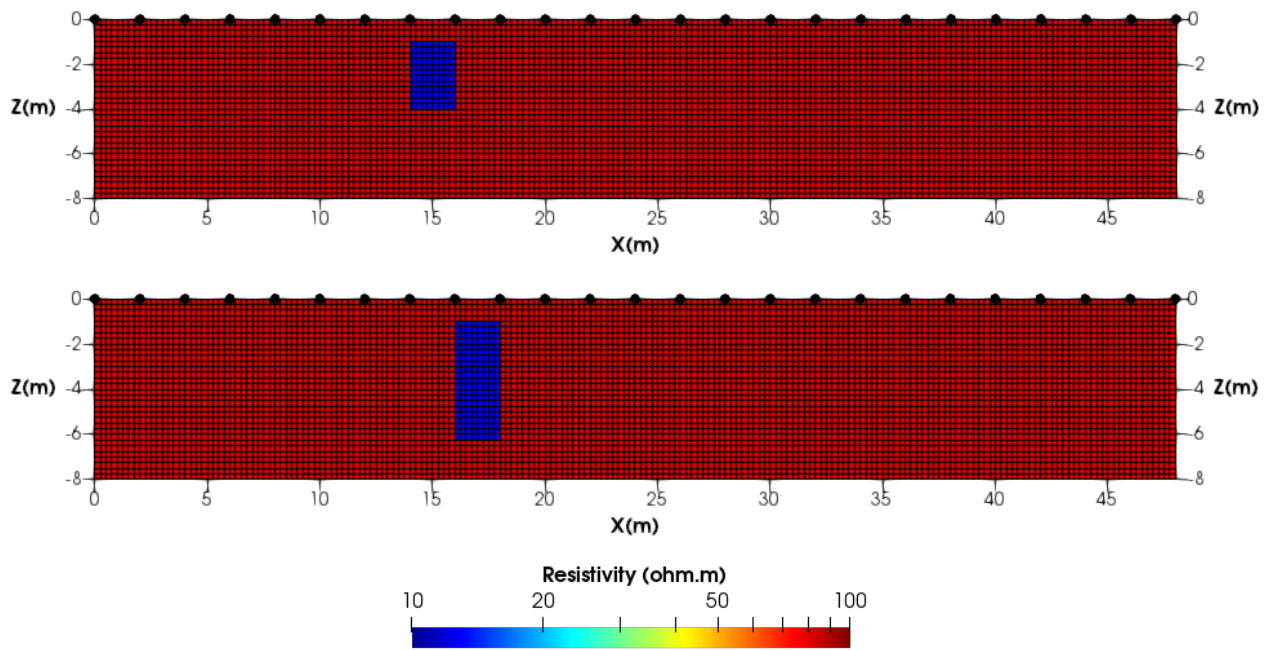


Figure 11.14. Forward model definitions for difference inversion example. The upper image is time 0; the lower image is time 1. (Plotted in *ParaView*, the grid shows the finite element discretisation).

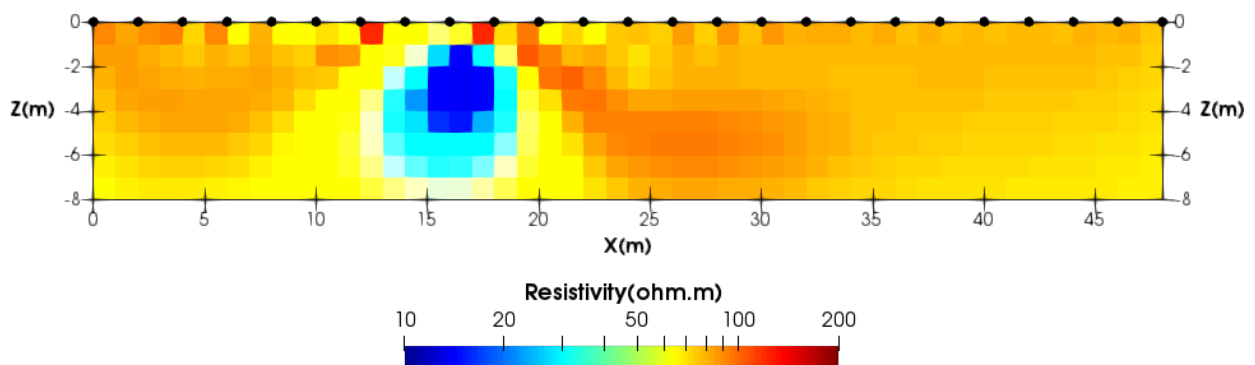


Figure 11.15. Resistivity model obtained from difference inversion (plotted in *ParaView*).

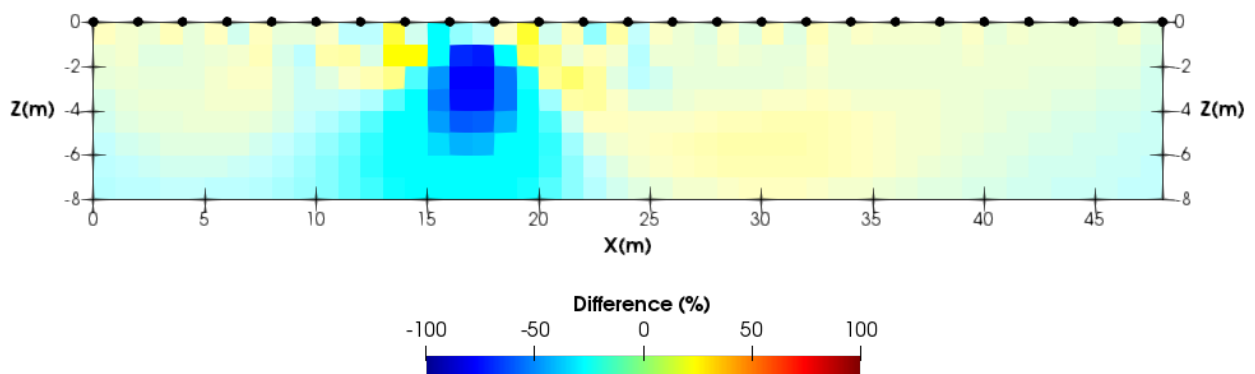


Figure 11.16. Change in resistivity from difference inversion (plotted in *ParaView*).

11.8 Surface electrode array 8 – triangular meshing

The folder Examples/Surface_8/ contains input files for running a forward and inverse problems for the dipole-dipole survey (from Surface electrode array 1) using a triangular mesh. The mesh is defined in **mesh.dat**. It contains 4,204 elements and 2,160 nodes. The region modelled extends approximately 200m to the left and right of the electrode array, and approximately 200m beyond the zone of investigation.

The folder Examples/Surface_8/Forward contains the input files for a forward model. In this mesh the first 40 elements represent the $10\Omega\text{m}$: in **R2.in** the two regions are defined. Figure 11.17 shows a plot of the forward model definition using *ParaView*. Note that the region extracted for plotting is based on the position of the centroid of elements and consequently a ‘jagged’ boundary often exists for triangular mesh output.

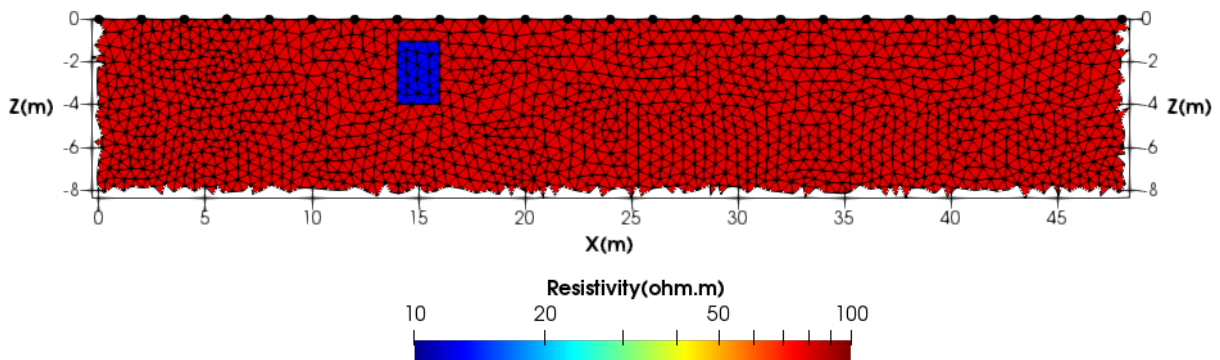


Figure 11.17: Definition of forward model using a triangular mesh

The folder Examples/Surface_8/Inverse_1 contains the input files for an inversion of the dipole-dipole data using a triangular mesh. Figure 11.18 shows the result, plotted *in ParaView*.

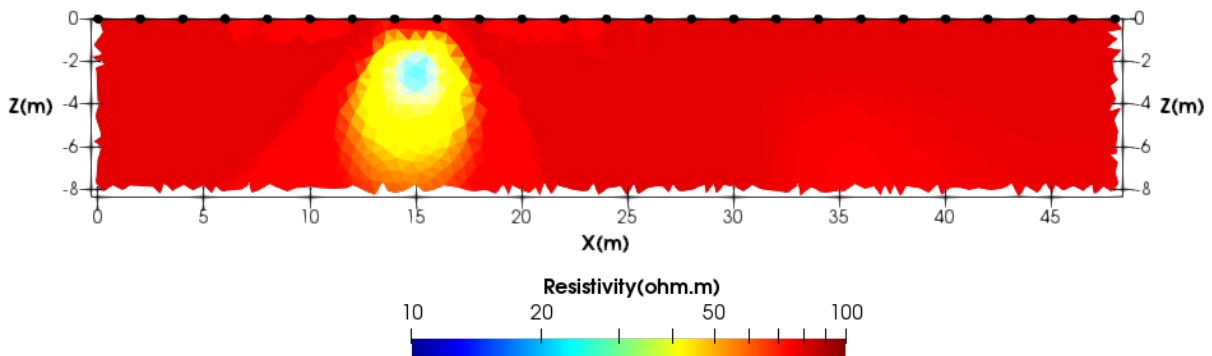


Figure 11.18: Inversion of dipole-dipole data.

The folder Examples/Surface_8/Inverse_2 contains the input files for an inversion of the same data using anisotropic regularisation to minimise lateral smoothing (see Figure 11.19).

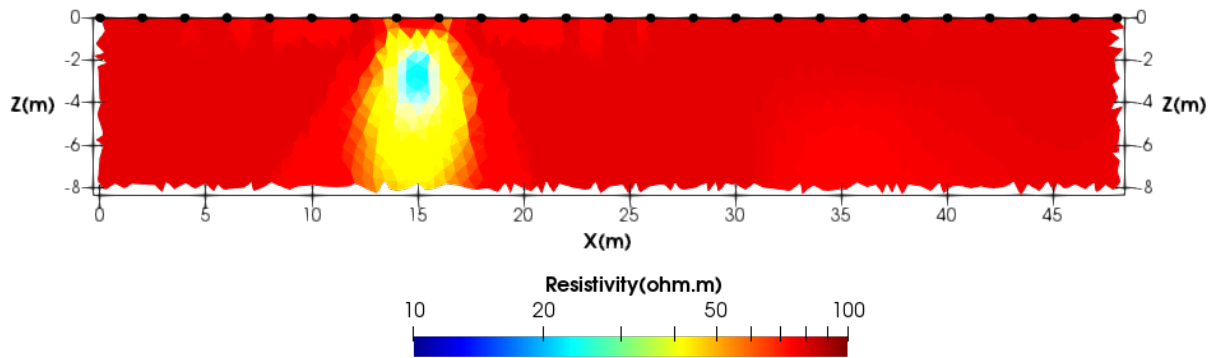


Figure 11.19: Inversion of dipole-dipole data with enhanced vertical smoothing.

The folder Examples/Surface_8/Inverse_3 contains the input files for an inversion of the same data as above but in this example the inverse region is blocked into two zones: one representing the low resistivity zone in Figure 11.17 and the other representing the remainder of the mesh. The inversion is shown in Figure 11.20. Note that although there is variation within each zone (since the same number of parameters exists), by defining the boundaries a near-perfect result is achieved (although this is a somewhat artificial case).

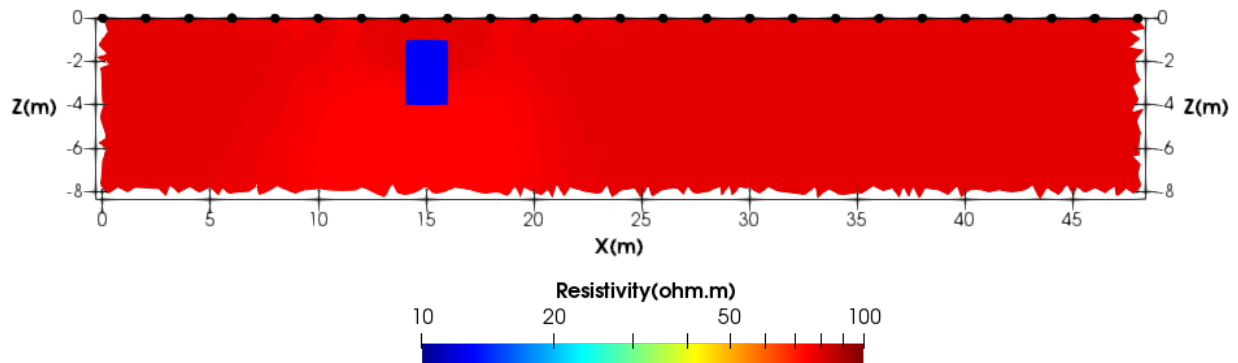


Figure 11.20: Inversion of dipole-dipole data with region blocking.

The folder Examples/Surface_8/Inverse_4 contains input files to illustrate the effect of fixing resistivity using a triangular mesh. In this case the starting resistivity is set to $20 \Omega\text{m}$ and 40 elements that occupy the area where the low resistivity feature exists are removed from the parameterisation by setting their parameter number to zero in **mesh.dat**. Note that to do this we have to move this block of elements in **mesh.dat** to the end of the list of elements (compare Examples/Surface_8/Inverse_4/**mesh.dat** with Examples/Surface_8/Inverse_3/**mesh.dat**). Since we have assigned parameter number zero to these elements then the resistivity remains fixed to the starting model ($20 \Omega\text{m}$) but all other elements can change in the inversion. Figure 11.21 shows the resulting inversion. Note that the true target is $10 \Omega\text{m}$ and so by forcing the region to be $20 \Omega\text{m}$ the adjacent elements are affected as the inversion compensates for the difference.

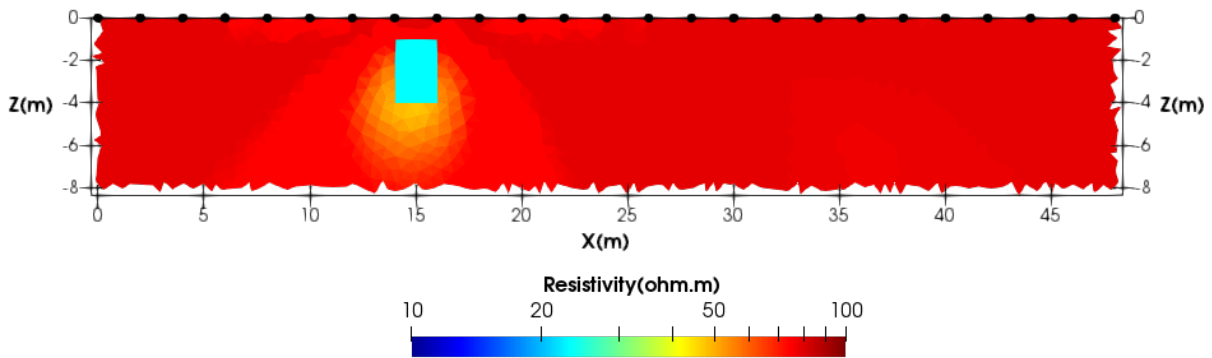


Figure 11.21: Inversion of dipole-dipole data with 40 elements (where the ‘target’ is located) set to 20 Ωm (the true value is 10 Ωm and so some smearing around the ‘target zone’ exists).

11.9 Surface electrode array 9 – quadrilateral mesh in **mesh.dat**

The folder Examples/Surface_9/ contains input files for running a forward and inverse problem when a quadrilateral mesh is read from **mesh.dat** (i.e. mesh type = 6). The example used here is the same setup as Surface electrode array 1 using a dipole-dipole configuration, but rather than defining a mesh in **R2.in**, it is read from the file **mesh.dat**. Figure 11.22 shows the inverse model. Clearly for this problem the use of a separate mesh file is unnecessary, but it allows the user to understand the way in which a pre-defined quadrilateral mesh can be used.

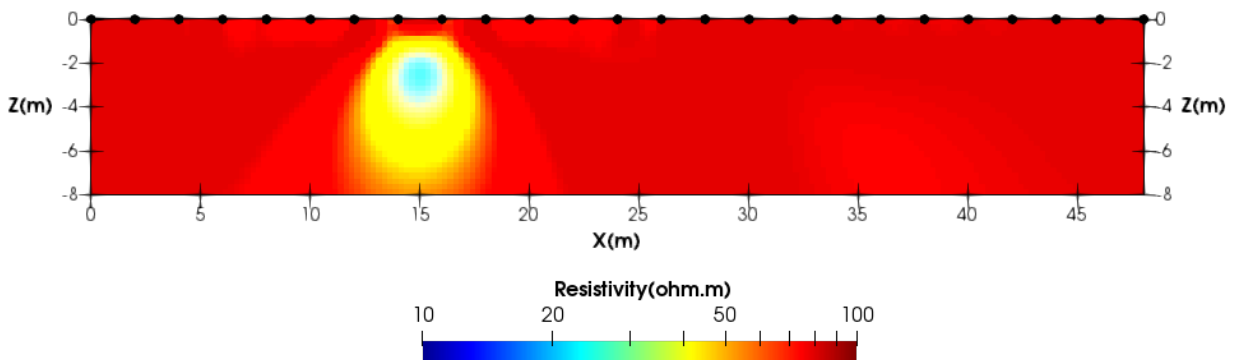


Figure 11.22: Inversion of dipole-dipole surface electrode data using quadrilateral mesh read from **mesh.dat**

11.10 Cross borehole array

The subfolder “Examples\Xbh” contains forward and inverse models for two cross borehole examples illustrated in Binley and Kemna (2005). The first case considered here is included in “Examples\Xbh\8m_skip7”. In this case measurements are made between two boreholes 8m apart, as illustrated in Figure 11.23. As in previous examples a zone with resistivity 10 Ωm is embedded in the 100 Ωm half space. The measurement scheme used is a “skip 7”: dipole – dipole with 7 electrode in between each current and potential electrode pair (see the **protocol.dat** file).

The forward model input files are included in “Examples\Xbh\8m_skip7\forward” and the inverse model files are in “Examples\Xbh\8m_skip7\inverse”. Figure 11.24 shows the output of the inverse solution using the forward model as “data”.

The second cross borehole case is for two boreholes 15m apart, as illustrated in Figure 11.25. The forward model input files are included in “Examples\Xbh\15m_skip7\forward” and the inverse model files are in “Examples\Xbh\15m_skip7\inverse”. Figure 11.26 shows the output of the inverse solution using the forward model as “data”. The effect of increased spacing of the boreholes on sensitivity of the measurements can be seen by comparing Figures 11.26 and 11.24.

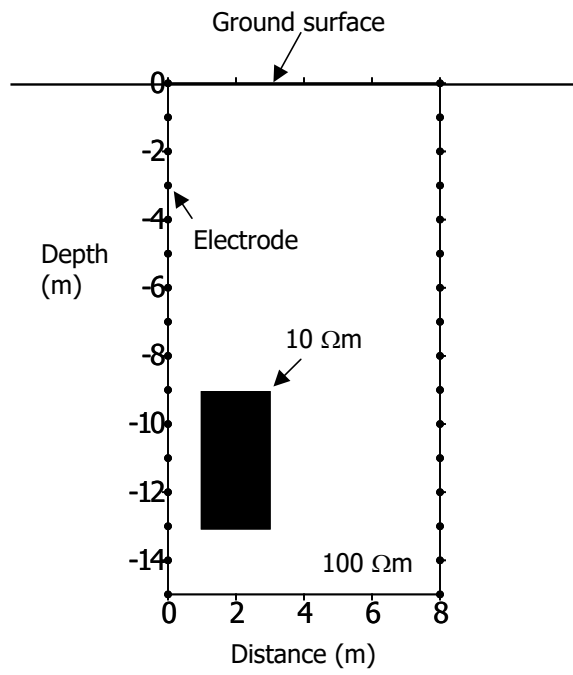


Figure 11.23: Forward model definition for cross borehole case 1

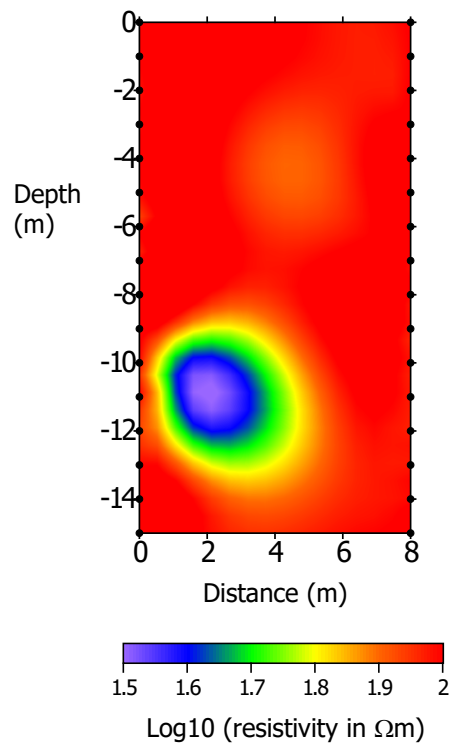


Figure 11.24: Inverse model for cross borehole case 1

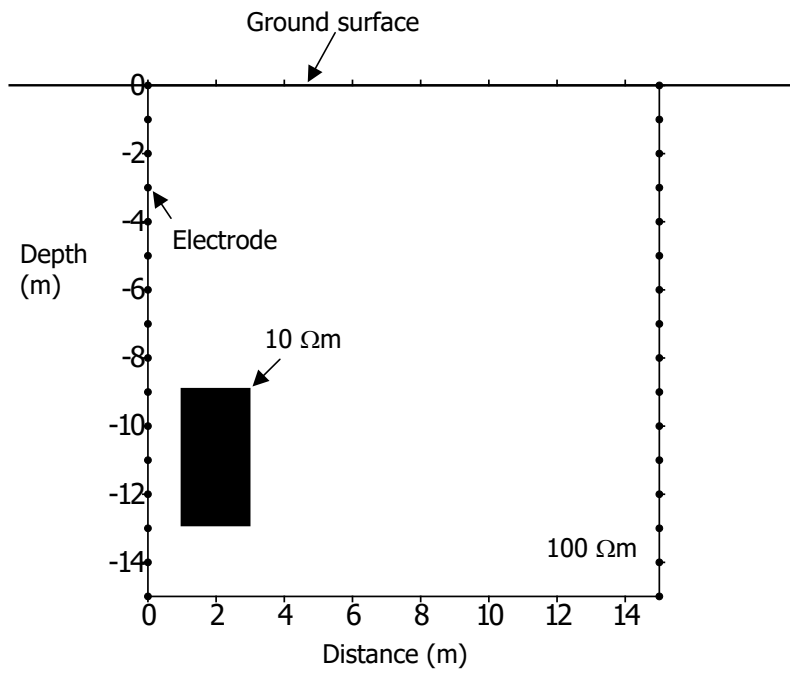


Figure 11.25: Forward model definition for cross borehole case 2

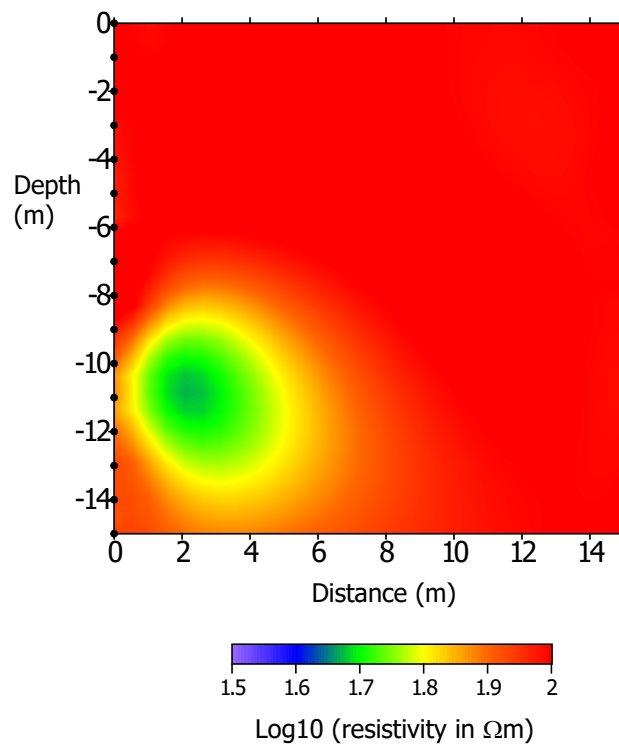


Figure 11.26: Inverse model for cross borehole case 2

11.11 Column model

The subfolder “Examples\Column” contains forward and inverse models for a simple circular arrangement of electrodes. In this example 16 electrodes are placed around the perimeter of a circular region (representing, for example, a soil column). In the forward model (see Figure 11.27) a 500Ωm circular target is placed in the 100Ωm vessel. The mesh in Figure 11.27 was used to compute the response of 103 measurements in a dipole-dipole configuration. The generated transfer resistance were then perturbed with noise with zero mean and a standard deviation related to the transfer resistance, R according to:

$$\sigma(R) = \sqrt{a^2 + b^2 R^2},$$

with $a = 0.001\Omega$ and $b = 0.02$.

These data were then used for the inversion with `a_wgt` set to 0.001 and `b_wgt` set to 0.02. Note that to avoid any bias in the modelling a different finite element mesh was used for the inversion, since the forward modelling mesh has a higher density of elements in the region of the anomaly in order to correctly place the anomaly in the mesh. In the inverse model mesh a more uniform triangular mesh is used. Figure 11.27 shows the inverse model for the problem.

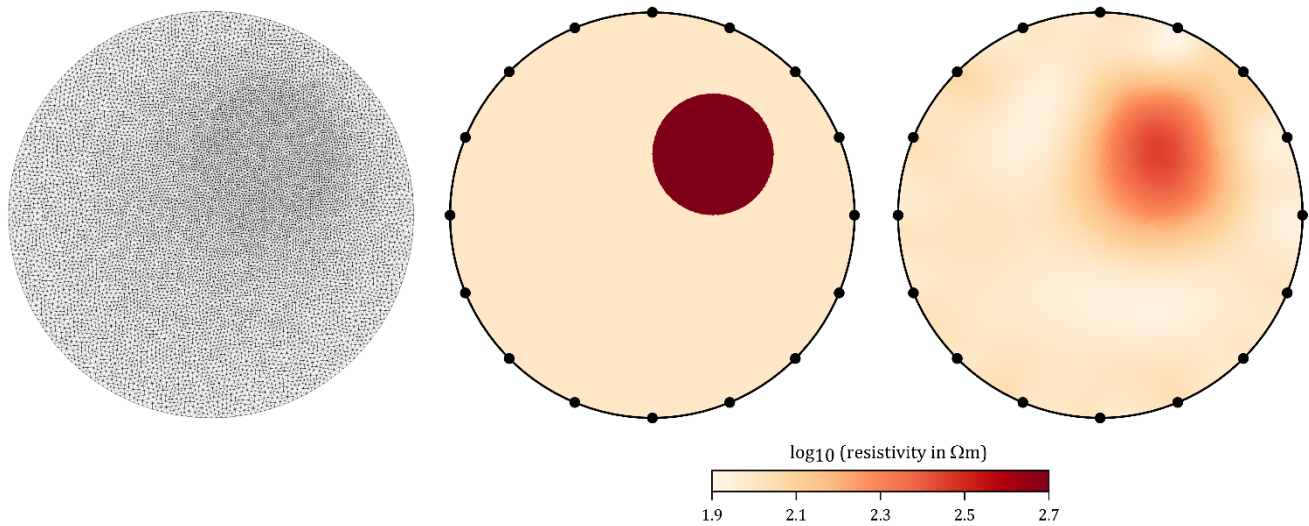


Figure 11.27: Column model example. Left hand image shows finite element mesh used for forward model. Centre image is the forward model. Right image is the inverse model.

12. Additional codes and scripts

The **R2** package contains a number of codes and scripts that may help the user in creating input files and visualising output from **R2**. Note that I have not tested any of these except the first set of mesh utilities. Some of these scripts may not be compatible with current versions of **R2** and Gmsh.

Meshing

Folder **Mesh_Uilities/Binley**

GenGmshGeo2D.exe

Creates a Gmsh geo (geometry file) which may be used for creating a triangular mesh. Note that the geo file can be edited before meshing, e.g. to add topography. The geo file created is **GenGmshGeo2D.geo**

GmshMsh2R2.exe

Reads the **GenGmshGeo2D.geo** created (and, perhaps, edited) in Gmsh, which can be meshed, creating a msh (mesh file) **mesh.dat**. Note that the first line will contain the number of elements, which is needed in **R2.in** for defining the resistivity (starting model or forward model definition).

Gen_R2in.exe

Reads a **ProfileR.in** file (see www.es.lancs.ac.uk/people/amb/freeware/profiler/profiler.htm) and creates an **R2.in** file for an equivalent mesh. This is useful for users moving from the simpler inverse code **ProfileR** to **R2**.

Folder **Mesh_Uilities/Boyd**

gmsh2R2msh

This python code and executable (written by Jimmy Boyd (British Geological Survey/Lancaster University)) will convert a Gmsh msh file to an **R2 mesh.dat** file.

Folder **Mesh_Uilities/Claes**

create_mesh

A Matlab script written by Niels Claes (Wyoming University) will create an **R2 mesh.dat** file for a triangular mesh.

Plotting

Folder **Plot_Uilities/Claes**

plot_resistivity

This folder contains a Matlab code for plotting output from **R2**, kindly provided by Niels Claes (University of Wyoming).

Folder **Plot_Uilities/Tso**

plot_resistivity

This folder contains a Matlab code for plotting output from **R2**, kindly provided by Michael Tso (Lancaster University). The code will plot different levels of transparency depending on the sensitivity map.

Complete wrapper (files not included but can be downloaded from links)

pyres

Kevin Befus (University of Wyoming) has produced a python wrapper for **R2** – see Befus (2017) and <https://github.com/kbefus/pyres>.

ResIPy GUI

Guillaume Blanchy (Lancaster), Sina Saneiyan (Rutgers) , Jimmy Boyd (BGS/Lancaster), Paul McLachlan (Lancaster/BGS) have developed an open source python GUI for **R2** and sister codes. See <https://gitlab.com/hkex/resipy> which also includes links for standalone executables. More information is also available at <https://resipy.org/>

13. Getting started with *ParaView*

The vtk files created by **R2** have been structured to work in **ParaView** - an open source visualisation application that can be downloaded from <https://www.paraview.org/> Users are advised to study online tutorials on **ParaView**. Here are a few simple tips to help the user get going.

The **fXXX_res.vtk** file contains the inverted resistivity, log transformed resistivity, a sensitivity map or resolution matrix (if selected) and a difference inversion (if selected). The file also contains the finite element mesh structure.

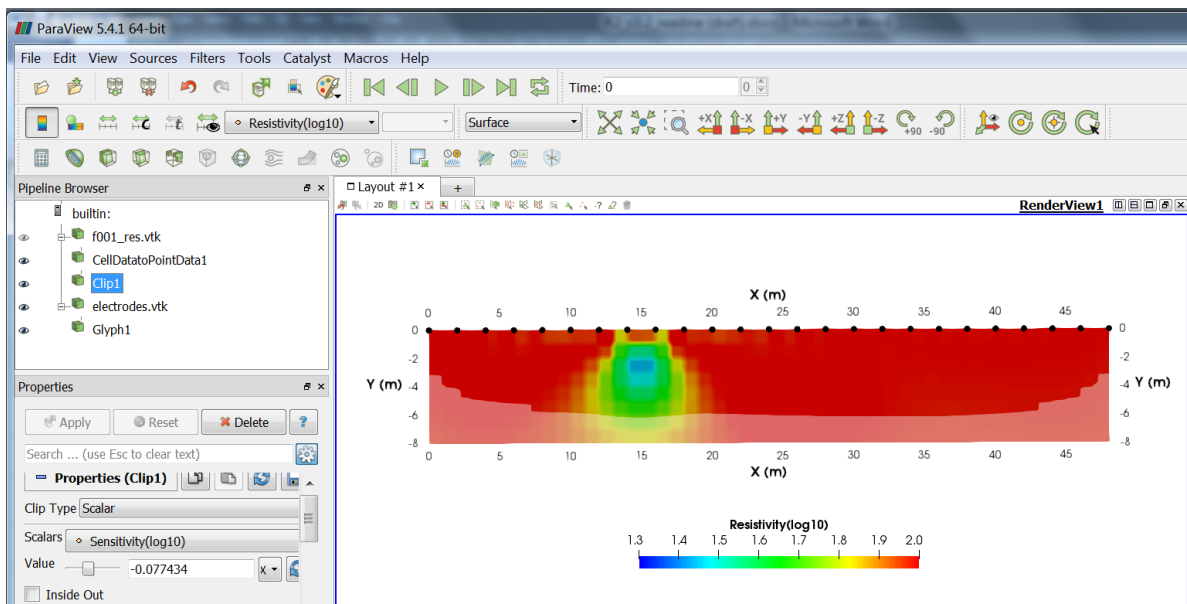
Open a **fXXX_res.vtk** file in **ParaView**, click **Apply** under **Properties** and you will get a map of the resistivity. Under **Coloring** in **Properties** you can select one of other variables stored, e.g. log10resistivity.

The default **Representation** of the image is **Surface**. Change to **Surface with edges** to see the finite element mesh and the resistivity image.

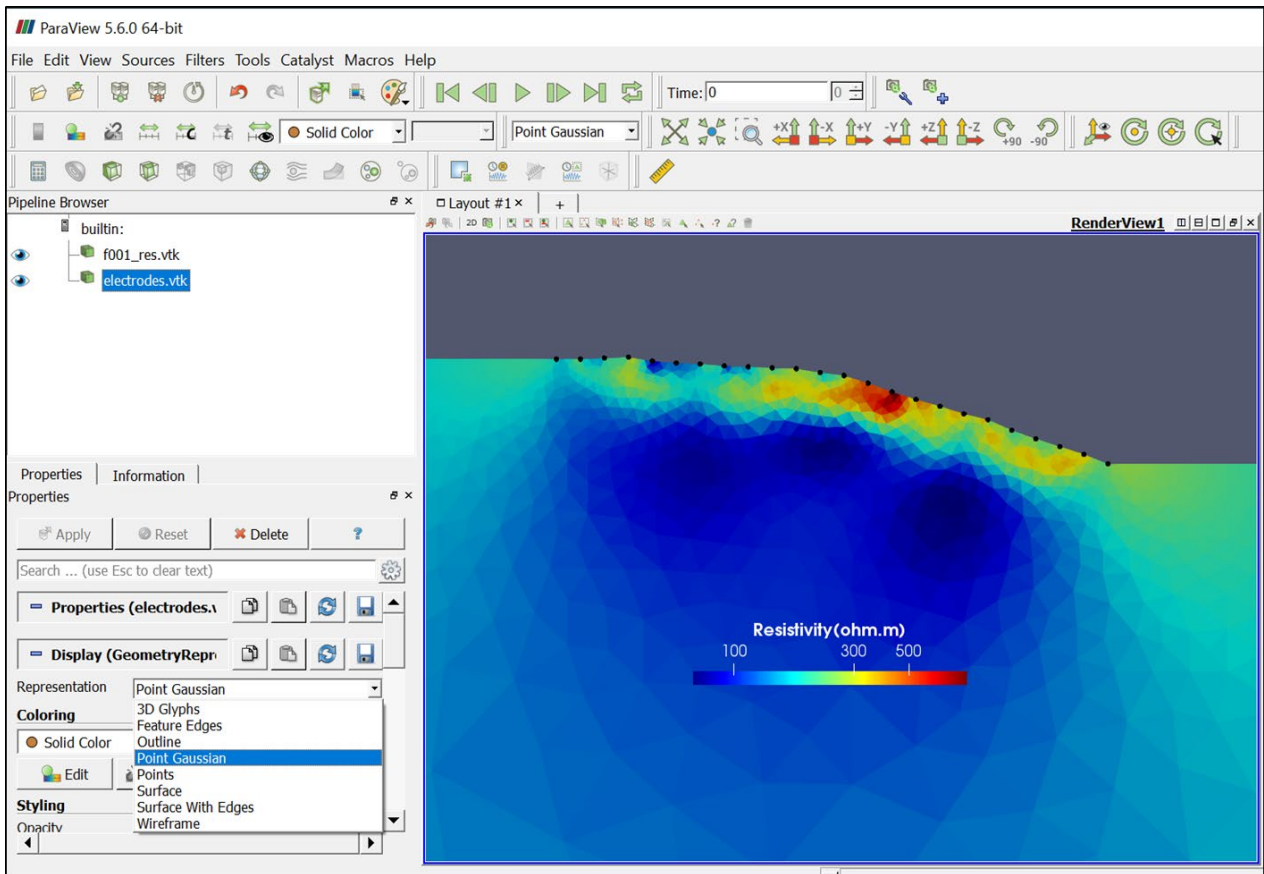
Axis labels and the colour legend are easily changed to suit the user.

To get an interpolated image (rather than one that shows element by element) then highlight the vtk file in the **Pipeline Browser** and select the **Cell Data to Point Data** Filter. Then select **Apply** in **Properties**.

If you want to show an image with thresholded values based on the sensitivity map then select an **Opacity** of 0.6 under **Styling** in **Properties**. Now select the **Clip Filter**. Select **Clip Type** as **Scalar** under **Properties** and select **Sensitivity(log10)** as **Scalars**. Select a mid-range value in the slider bar for **Value**. Under **Coloring** select **Resistivity(log10)**. You should now see the thresholded region as a solid colour and the outer area as opaque (see figure below).



To show the electrodes, open the **electrodes.vtk** file and click **Apply** under **Properties**. Now select the **Glyph** filter and under **Glyph type** select **Sphere**. Make the radius of the sphere smaller than the default, say 0.05, and select **Apply**. You can change the colour of the glyph in the **Properties** box. If not all electrodes are displayed then select **Masking** under **Properties** and select **Glyph mode** to **All Points**. I have noticed in recent versions of Paraview that Glyph plotting sometimes does not show all the points. This appears to be a bug in recent Windows versions of Paraview. If this occurs then you can show electrodes positions by simply selecting the properties type of **electrodes.vtk** in **Paraview** to **Point Gaussian** (see example below).



14. Common user errors

Below is a list of some common user errors that I have encountered. This may be useful for new users.

A common mistake is for a new user to go straight into trying to run an inverse solution without getting a good feeling for the model that is being used. New (and old) users working on new problems should first try run a forward model for a uniform resistivity. This will help sort out any problems with the definition of the mesh, etc. It will also be useful in understanding the quality of the forward model and help judge this against the quality of the data.

If you can, run the code from the command line. You will need to run CMD in Windows, then move to the correct folder and then type **R2**. Doing it like this help see any errors if the program crashes unexpectedly because of incorrect input.

In the example input files provided there are comments at the end of most lines in the form “<< comment”. Note that these are always at the end of a line. You cannot have these appearing on their own in a line. If you do then **R2** will try read this comment when it is expecting numerical input and simply crash.

The mesh is based on elements and nodes. In **R2.in** Lines 3 to 9 are based on nodes, whereas Line 13 is based on elements. It is important to understand the difference and not mix the two.

On Line 22 in **R2.in**, specifying a tolerance of 1.0 means that you are happy that you have estimated your errors correctly (Line 23). Don't just use the `a_wgt` and `b_wgt` values in the example files – spend time to understand the likely errors in your measurements and model.

Setting `data_type` to 1 in Line 22 of **R2.in** means that the data you input will be log transformed in **R2**, not that you have to supply logged data. You must specify the polarity of the data, as always.

Setting the minimum and maximum apparent resistivity (Line 23 of **R2.in**) is only valid if you have a flat surface and an infinite half space problem, otherwise the geometric factors that **R2** will compute will be incorrect.

For a structured quadrilateral mesh the electrode positions are defined by their column and row positions in the mesh (Line 27 of **R2.in**). These are not the co-ordinates of the electrodes but their position in the mesh.

In the definition of the input files, each line has been defined in terms of the type of numbers that are required. For example, (Real, 2 Int, 2 Real) means one real number, followed by two integers, followed by two reals. You can substitute integers for reals but not the other way round. So if the code is expecting an integer and your line entry has 1.3, for example, then the code will crash.

Note that the data in **protocol.dat** should be provided in transfer resistances, NOT apparent resistivities. Also note that the polarity should be retained in the data. It is very wise to check the polarity of your measurements – you can do this by computing the geometric factor for your measurement configuration (provided topographic and non-infinite boundaries are not significant). If you don't know how to compute the geometric factors then you should run a forward model with **R2** for a uniform half space and compare the computed polarities with those in your data. For a surface electrode array your data should be the same polarity as the model, otherwise the measurements will not be included in the inversion. For electrodes not on the surface the polarity can change as the resistivity structure changes in the inversion.

Make sure you check that the solution has converged in inverse mode (see **R2.out**). Just because a resistivity model has been computed it does not mean that convergence has been reached. If the solution has not converged then go through the **fxxx_err.dat** file and look at see if any particular

measurements are problematic. Also check that you are confident with the `a_wgt` and `b_wgt` error settings you have applied (Line 23, **R2.in**). A common mistake is to set these too low. A good estimate of `b_wgt`, in particular, is important. Normally, you should be able to get convergence in less than 5 iterations. It is not wise to increase the maximum number of iterations to a large number. If you don't get convergence in 10 iterations then there is definitely some problem with the data, the assumptions or the input files.

14. References

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