Scottish COVID-19 Response Consortium

Monday, 27th July 2020





Network Simulation

Jess Enright (Glasgow) Bob Turner (Sheffield) Rafael de Almeida (Man Group) Chris Hughes (Man Group) Fedor Gorokhovik (Man Group)

Language	Python
Spatial scale	Data dependent – currently Health Board or IZ
Model type	Spatially-embedded network of age-structured populations, deterministic or stochastic, compartmental model
Features	 Movement flows from data or simulated Age-class mixing from input matrix Local and long-distance spread Dynamic movement and contact damping
Mode	Forward simulation, daily timesteps Basic inference implemented – ABC-SMC

Key questions

- Control related to age class or movements

- Importance of network flows, impact of changes to flows

https://github.com/ScottishCovidResponse/simple_network_sim

Will Pettersen (Glasgow) Anthony O'Hare (Stirling) Leighton Pritchard (Strathclyde) Alex Konovalov (St Andrews) Jason Dykes (City) Jo Wood (City)





Network Simulation

<u>https://github.com/ScottishCovidResponse/simple_network_sim</u>

Significant achievements over the RAMP period

Software engineering	Many major improvements in design, automated testing, documentation, reproducibility, and more!
Modelling functionality	 Choice to focus on network-of-populations Generalisation to arbitrary regions given data Generalised compartmental model Time-varying activity damping Stochastic model operation Generating realistic behaviour Enormously improved software choices!
Data Interface	 Move to inputs from files instead of hard-coded or simulated Using real data as input Data Pipeline API integration
Inference and Sensitivity	 Linear and non-linear sensitivity analysis Implementation of ABC-SMC for basic inference



Contact Tracing

Sibylle Mohr, Louise Matthews (EPIC / Glasgow)



Sam Brett, Vino Mano (Man Group), John Nonweiler (UKAEA), Ed Townsend

https://github.com/ScottishCovidResponse/Contact-Tracing-Model

Language	Java
Spatial scale	No explicit spatial scale but a form of 'location' is retained
Model type	 Individual-based stochastic network model Age-structured individuals Weighted contacts
Key Feature	Flexible contact tracing scenarios
Mode	Forward simulation, user-defined timesteps (quarter of day)

Key questions

What are the optimal contact tracing protocols?

- Benefits of blanket vs tailored actions and advice for alertees?
- How can we reduce the burden of contact tracing whilst maintaining high levels of efficacy
 - Targeted alerts / rapid testing / release of contacts from isolation
- How much more effective does the tracing become if tracing of secondary contacts is allowed?
- What is the impact of basing alerting on a positive test rather than symptoms?





Contact Tracing: Key features

Sibylle Mohr, Louise Matthews (EPIC / Glasgow)



Sam Brett, **Vino Mano** (Man Group), John Nonweiler (UKAEA), Ed Townsend

Explore contact-tracing policies

Isolation measures

Blanket 14-day isolation vs. dependent on the time of contact (0-14 days)

Alerts / testing

- targeting of alerts at individuals most likely to be infected
- testing of individuals to release their contacts from isolation

Different 'alerting' scenarios

- Alerting based on symptomatics
- Alerting based on positive test

Contact tracing

- Direct contacts only
- Also secondary contacts (contacts of direct contacts)





RSE core team	Sam Brett Vino Mano (Man Group) John Nonweiler (UKAEA) Edward Townsend
Inference / model assessment	Rikiya Takahashi Fedor Gorokhovik (Man Group)
Visualisation team	Cagatay Turkay (Warwick) Dan Archambault (Swansea) Kai Xu (Middlesex)
Contact tracing options	Louise Matthews (UoG) Jamie Prentice (UoG)

Contact Tracing Team

Major RAMP Achievements

Software development

- Code clean-up; codebase tested / integrated / optimised; re-factoring; added software tests / unit tests...
- Documentation, verification, integration into the SCRC environment...

Model functionality

- Multiple, sophisticated contact-tracing scenarios / secondary contacts / global lockdown policies / testing scenarios / test efficacy
- Model runs on various contact data, together with list of agestructured individuals; Random infection / targeted seeding
- Complex statistics output (R calculations; traced / isolated / infected...) Inference
 - Sensitivity analysis for model parameters / policy parameters
 - Comparison between CTM model and ODE model

Visualisation

- Multiple static and dynamic visualisation of different output data
 - Network data / compartmental outputs / infection maps

And so much more!!

• Data API for Java is taking shape; new documentation / inferences / visualisation...



Spatial Simulation

Claire Harris (EPIC / BioSS) R0 →

https://github.com/ScottishCovidResponse/Simulation.jl

Language	Julia	
Spatial scale	1 km ² grid, Scotland / UK	/
Model type	Explicitly spatial, stochastic, compartmental model	
Features	 Airborne and environmental spread of virus Local spread vs. long-distance commuting Impact of climate / environment on transmission Demographic structure, population density Inference and visualisation frameworks 	
Mode	Forward simulation, daily timesteps	Ъ К



ISSUES HPC THREADING

RSE team: Alex Robson, Bella Wu, Eric Perim Martins and Sean Lovett (Invenia)

James Cook (UKAEA)





Inference: Ben Swallow and Simon Babayan (Glasgow)



Visualisation: Aidan Slingsby (London City)



Data: Sonia Mitchell and Ciaran McMonagle (Glasgow), Stephen Catterall (BioSS) and Jeremy Walton (Met Office)

Key questions

- What effect does long term pollution have on susceptibility / severity of COVID-19?
- What is the effect of weather/environment on the virus? ٠
- What are the relative contributions of direct/indirect transmission? •



Spatial Simulation

Claire Harris (EPIC / BioSS)



https://github.com/ScottishCovidResponse/Simulation.jl

Major developments

- Codebase:
 - Integrated, tested, documented, optimised
 - Python wrapper for data pipeline
 - Fully deterministic version of code
- Epidemiology:
 - Mostly everything!
- Data:
 - Data flowing from the pipeline
 - Demographics/Epi params/Weather/Pollution
- Inference:
 - ABC-SMC interface in R that can recover initial parameters
- Visualisation:
 - Fully interactive Java visualisation, with multiple modes, scaling and spatiotemporal dynamics





Individual-based Simulation

Paul Bessell (Edinburgh),



John Nonweiler (UKAEA), Blair Archibald (Glasgow), Bob Taylor

https://github.com/ScottishCovidResponse/Covid Simulation Model

Language	Java				
Spatial scale	Defined area (eg Lothian HB, Orkney)				
Model type	Individual-based stochastic simulation				
Features	 Individual hourly movements and mixing Implicit network structure Full age and household structure Mixing and transmission in distinct community compartments Health boards and care homes 				
Mode	Forward simulation, hour time steps				
Fitting	Relies on parameters and visual comparison to data				
Data	Most key parameters are now evidenced, but would be good to complete the list				

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Model purposes

- Detailed simulation of different communities
- Completely flexible reopening/reclosing of businesses and compartments of society
- Comparison between different communities / areas
- Scenarios for opening schools
- Flexible addition of new societal compartments (could add theatres, cinemas etc)
- Shielding populations
- Strategies for roll-out of vaccination or new tests
- Role of superspreaders
- Informing other models with network structure



Individual-based Simulation



Major RAMP Achievements

Software development

- Simple terribly written code has been transformed into a very efficient and complete epidemiological model
- Complete testing environment with the model
- 1 run of a 200 day simulation of 910,000 population on DiRaC is ${\sim}22~\text{mins}$
- Full software documentation

Model functionality

- Fully age structured disease progression
- Age structured household structure and implicit contact network
- Fully age-structured non-Covid hospital utilisation
- Disease transmission during travel
- Build-your-own lockdown release scenarios

Fitting

- (For Lothian at least) Model broadly fits the mortality, hospitalisation and R values)
- Will run it through Thibaud's model

Further steps

- Write up the epidemiological documentation
- Get better contact parameter data



ABC-smc

Thibaud Porphyre (Edinburgh)



Peter Fox (UKAEA)

https://github.com/ScottishCovidResponse/Covid19 EERAModel

Language	C++
Spatial scale	Flexible
Model type	Age-structured compartmental stochastic model
Features	 Different transmission behaviour between community and HCW Impact of bed capacity on hospitalisation rate
Mode	Inference – ABC-smc Forward simulation

Model purposes

- Inference of key epidemiological parameters
- Impact of scales (national vs regional vs health board)
- Prediction of community level infection
- Quantification of number of primary infection
- Optimization lifting movement restrictions strategies





RSE team: Sanket Gadgil, Kristian Zarębski, Qingfeng Xia (UKAEA), Andy Bennett

Epidemiology: Mark Bronsvoort, Paul Bessell (Edinburgh), Louise Matthews (Glasgow)



Uncertainty quantification: Ben

Swallow (Glasgow), Ian Vernon (Durham), and the rest of #UQ team



Data: Stella Mazeri (Edinburgh)







ABC-smc

Major RAMP Achievements

Software development

- Simple terribly written code has been transformed into a very efficient and complete epidemiological model
- Complete testing environment with the model
- Full software documentation
- Full epidemiological documentation
- Sensitivity analysis

Model functionality

- Both inference and forward preduction implemented
- Fully age structured disease progression
- Role of HCW in the case reporting

Fitting

- Model broadly fits the mortality, hospitalisation and R values for Scotland
- Inference framework validated

Further steps

- Uncertainty quantification
- Coding and assessing lockdown strategies
- Fit on all health board in UK



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Chris Pooley (BioSS / EPIC) Glenn Marion (BioSS/ EPIC)

https://github.com/ScottishCovidResponse/CoronaPMCMC

Language	C++
Spatial scale	Middle Layer Super Output Areas (MSOA) or output areas (OA), Scotland
Model type	Individual-based, spatial, stochastic compartmental model
Features	 Individual risk factors, e.g. age, gender Area risk factors, e.g. population density Time variation in transmission Calculation of model evidence (ME) Optimized parallel implementation
Mode	Inference using multi-temperature MCMC with model based proposals

Key questions

- How is R changing as a function of time?
- What determines the spatial spread of disease?
- What are the effects of government policies?



lan Hinder (Manchester) Robin Williams (Bristol)

 Data: Richard Bailey (Roslin) Stephen Caterall (BioSS)
 Model: Glenn Marion (BioSS) Andrea Doeschl-Wilson (Edinburgh





Model parameter inference

- Data: National hospital admissions /populations and regional death data.
- Distributions for certain transitions.

To Do...

- Comprehensive validation.
- Results for age structured populations with sex.
- Incorporation into data pipeline.

Variation in R

 Captured time variation in disease transmission before/after lockdown.

Population density

- Higher disease transmission in areas of high population density

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Frequency dependent

Density dependent

- Different area factors, e.g. deprivation, pollution.
- Sensitivity analysis.
- Use model evidence to identify best available model for Covid-19 in Scotland.

Requirements

- Reproducible
- Traceable
- Validated
- Open source
- Open data

Open Epidemiology

Requirements

- Reproducible
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Open Epidemiology

https://github.com/ScottishCovidResponse

Alys Brett (UKAEA)

Enabling software teamwork

Team processes: Lead RSEs

Collaboration infrastructure: Andrew Lahiff, Jonathan Hollocombe, Nathan Cummings (UKAEA). Collaboration: everyone!

Zulip chat:

Now reached >5000 weekly messages

Software Quality

• Improving code clarity and software structure

Alys Brett (UKAEA)

• Automated testing and code analysis

Documen	tation		
Model Overview	Doxygen Code Documentat	ion	
Code Che	ck Reports		
Flawfinder Cla	ing Tidy Code Coverage	CPP Check	Sim C++
Builds			
Branch	s	tatus	
master	۵	Covid19EERAMoo	del no status
dev	[C	Covid19EERAMoo	del passing

COVID-19 EERA Model

This is the documentation website for the EERA COVID EERA Model repository on GitHub.

Showing min	in per day coverage for the last 6 months						
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Alys Brett (UKAEA)

Improving reproducibility and trust

- Data pipeline integration
- Managing configuration, randomness, build, release run processes

Software Checklist

https://github.com/ScottishCovidResponse/SCRC-internal/blob/master/software_checklist.md

- Framework for evaluating software engineering aspects of model readiness
- Completed for current status of all models

Alys Brett (UKAEA)

Simple Network Sim

- Synchronised docs and code using docstrings & typehints to making it easy to get into the codebase
- Extensive automation of unit and regression tests and code-checking through CI lets us focus on adding features and fixing bugs
- Adopted industry standard Python data science tools `pandas` and `numpy` - peer-assured variable-types and functions
- Tight control of execution using `conda` virtual environment to help ensure reproducibility
- Great multidisciplinary working and input to current code from a range of contributors: academics, quantitative researchers, postdocs, engineers

Simulation.jl

- Software teamwork practices (first multi-developer team)
 - Issue boards & labelling, contribution and review guidelines etc
- Automated testing
 - Travis & Appveyor for Cl
 - Codecov for test coverage
- Extensive testing of new epidemiology code
- Reproducibility improvements
 - "Deterministic hijacking" of the stochastic model to allow regression testing
 - Run scripts, TOML files for code & dependancy versions
- Self-contained example run scripts serve as end to end tests
- Integration of data pipeline

Alys Brett (UKAEA)

Contact Tracing Model and Covid Simulation Model

- Many model refinements and new features
- Initial code clean-up then incremental improvements to design & implementation
- Automated tests and Cl
 - 90% unit test coverage, regression tests, basic automated epidemiological/model-validation tests
- Documentation for user, developers & to understand algorithms
- Improved reproducibility and trustworthy results
 - refactoring RNG usage
 - moving parameters to an input file, adding logging of git hash and inputs
 - R scripts for validation, version numbering and release processes
- Enabled **parallel runs** of models on DiRAC HPC
- Implementing the Java data pipeline
 - Close to end-to-end model run (using CSV instead of HDF5 files initially)

Alys Brett (UKAEA)

New functionality: Multiple model structures, forward prediction / parameter inference modes

Reproducibility: Parameterised config of random number generation, Logging inputs, outputs, versions

Software engineering and code quality

- Extensive refactoring and architecture improvements ٠
- CMake **build system**
- Unit and regression test frameworks ٠
- **Clautomation** of: tests, documentation generation (Doxygen), ٠ code coverage, static analysis
- Created **project dashboard** ٠ https://scottishcovidresponse.github.io/Covid19 EERAModel

Ian Hinder (Manchester)

- Development of C++ interface to Python **data pipeline** code, and integration with model (in progress)
- Fixed configuration in header files replaced with TOML configuration file
- Storing code **provenance** information and making runs reproducible
- Improved **code structure**, i.e. making it more modular
- Implemented CI (automated testing), as well as regression testing (flag whether a code change affects the numerical results)
- Added automated source code analysis to catch bugs found several

RSE – External Models

Alys Brett (UKAEA)

Peter Hill (York)

Imperial CovidSim Model

C THREADING

Integration with SCRC data pipeline

- Via a Python wrapper layer using pipeline API
- No need to touch original code
- Can treat chosen version as a black box whilst verifying inputs & outputs

LSHTM Model

Kristian Zarebski (UKAEA)

- Rationalised parameter initialisation
 - external config at start of run
- Faster runs with single scenario selected via parameter
- Integration with the SCRC data pipeline
 - R frontend for python to interact with pipeline API
 - Inputs converted to HDF5 & TOML now moving to data pipeline locations
- Collaboration with Swansea RSEs

Ruth Dundas (UoG), Iain McKendrick (BioSS)

Initial specification of Data Registry: with Aaron Reeves (SRUC)

Specification of data and metadata workflows

Literature review: procedure and associated data extraction tool

Dataset assessment: 'intrinsic quality', 'representativeness' and 'fitness for purpose' assessment procedure

Meta-analysis and distribution analysis: Jim Lewsey, Houra Haghpanahan, Ryan Field, Janine Illian, Caitlin Fox, Mahi Siddika, Megan Laxton, Martje Rave

Data brokering: Richard Bailey, Ciaran McMonagle

Specialist Dataset expertise: Ruth, Ciaran, Jeremy Walton, Denise Brown, Stephen Catterall, Amira Elayouty

Data source and provenance IDing and wrangling: Sonia Mitchell, Ruth, Ciaran, Denise

Data team: Richard, Ciaran, Sonia, Ryan, Jeremy Gribble, Hannah Jevans, Nardus Mollentze, Denise

Data pipeline

https://github.com/ScottishCovidResponse

- Reproducible
- Traceable
- Open source
- Open data

API

- C/C++
- Java
- Python
- Julia
- R

Data and metadata flow

- · · → Enter source data into pipeline
 - -> Download inputs to model
- ••••• Run model using Data Pipeline API
- - - Upload outputs to pipeline

Sonia Mitchell Ciaran McMonagle Nardus Mollentze Ryan Field

Data pipeline for input

https://github.com/ScottishCovidResponse/SCRCdataAPI
https://github.com/ScottishCovidResponse/SCRCdata

> 31,000 papers uploaded to the registry

8 data products uploaded to the registry

4 upload templates

Working on processing additional data products, generating upload templates, and checking robustness of code

GITHUB ISSUES HPC THREADING

Data pipeline for modelling

Richard Blackwell, Chris Hughes, Vino Mano, Rafael de Almeida (Man Group), Ian Hinder (Manchester), Kristian Zarębski (UKAEA), Alex Robson, Sean Lovett (Invenia)

https://github.com/ScottishCovidResponse/data_pipeline_api

Data registry

Jonathan Hollocombe and Andrew Lahiff (UKAEA)

https://github.com/ScottishCovidResponse/data-registry

- Available at data.scrc.uk
- Provides web-page view of stored data and information about registry API.
- API can be seen at data.scrc.uk/api
- More info available at data.scrc.uk/docs

SCRC data registration and management system Links * Logged in as: jholloc logout						
Home						
Data Products						
Namespace $ end{tabular}$	Name	Version \$				
EERA	fixed-parameters/K	0.1.0				
EERA	fixed-parameters/T_hos	0.1.0				
EERA	fixed-parameters/T_inf	0.1.0				
EERA	fixed-parameters/T_lat	0.1.0				
EERA	fixed-parameters/T_rec	0.1.0				

K Control

Epidemiology

Louise Matthews (Glasgow / EPIC)

https://www.gov.ie/en/publication/dc5711-irish-epidemiology-modelling-advisory-group-to-nphet-technical-notes

Inference and model assessment

Glenn Marion (BioSS / EPIC)

Inference: quantify epidemic and effect of interventions

- focus on simulation-based methods (model agnostic + parallelisable)
- But also data-augmentation MCMC methods (BEEPmbp)

MCMC

And emulation for Uncertainty Quantification and model fitting

Model assessment: better models

A key issue moving forwards

- statistical fit (evidence, residuals, DIC etc.) and predictions
- model misspecification
- validation within and btw model/code-base

Now in more detail from

- Ben Swallow (UoG)
- 🖵 Rikiya Takahashi and Fedor Gorokhovik (Man Group)

Inference* + SA > quantify uncertainty > model assessment > better models *<u>focus on</u> Bayesian inference

Inference and model assessment

Barves THAM JF Ben Swallow (UoG)

Inference: quantify unknown epidemiological parameters

- Again focus on simulation-based methods (easily(?) parallelisable)
- Uses an ABC-SMC algorithm to estimate 6 parameters on 1km² grid of Scotland
- quantify uncertainty in model output and parameters
- Flexible to varying data outputs and thresholds

MGMO

Model testing

- Using data from model simulations at known parameter values we are able to retrieve the true values
- Stochastic model so repeated runs at the same parameter values
- <u>Tested and seems all parameters retrieved using either deaths or</u> <u>symptomatic cases</u>

Issues/open questions

- Link to data pipeline
- Incorporate priors beyond uniform
- Consolidate multiple compartment summaries

Bayesian inference: simulated data

Red solid line = true parameter value Blue dashed line = posterior mean

Inference and model assessment

Rikiya Takahashi and Fedor Gorokhovik (Man Group)

Sensitivity Analysis

- Reparametrisation of exposure-related disease parameters in Contact Tracing Model
- Non-linear regression and SHAP analysis for total number of death and peak number of severely symptomatic persons
 - SHAP: SHapley Additive exPlanations (Lundberg & Lee, 2017)
- Efficient frontier in optimisation of the policy parameters under uncertainty

Open Issues Real-data-based posterior in policy optimiser, distributional policy parameter recommendations instead of point estimates

Inference

- ABC-SMC used to infer infection probability and initial infections in Simple network sim (contact multipliers to come)
- To be used in conjunction to stochastic mode to have more realistic posterior std dev
- Fitted on historical death per healthboard in Scotland
- Other parameters sources from external sources to be as credible as possible
- Wide priors chosen from Beta, Lognormal distribution

Open Issues Improved rejection mechanism, parallelization of inference

How Interaction with exposure exponent Affects total death

- 0.10 🖻

0.08 0.06 0.06 0.04 vuqom infect

S. M. Lundberg & Su-In Lee, A Unified Approach to Interpreting Model Predictions, NeuIPS 2017.

Dr. Rita Borgo, KCL

Elif Firat, Nottingham Dr. Radu Jianu, City

VIS

27 VIS/VA volunteers, plus Min Chen (Oxford U.)

Benjamin Nash Dr. Phong H. Nguyen, Red Sift Ltd. Dr. Helen C. Purchase, Glasgow Dr. Dylan Rees, Swansea Dr. Panagiotis Ritsos, Bangor Professor Jonathan Roberts James Scott-Brown, Edinburgh Dr. Aidan Slingsby, City Dr. William Teahan, Bangor Dr. Thomas Torsney-Weir, Swansea Dr. Cagatay Turkay, Warwick

Dr. Franck Vidal, Bangor Qiru Wang, Nottingham

Tianci Wen, Bangor

Professor Jo Wood, City Dr. Kai Xu, Middlesex

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VIS

27 VIS/VA volunteers, plus Min Chen (Oxford U.)

https://github.com/ScottishCovidResponse/rampvis-ui

rampvis-api

scrc-vis-analytival scrc-vis-modelling

Level 2. Analyti atlan, which is an investigative all for enamand ratio line, etc.). Despite the advancement of data in thing technology, nor requirements analysis shows that more modeling sciencies and epidemiolog ees to data seliding algorithms, such as its everyse analysis, clee e etmaalbaation beske sigare blaat annen paar y warb data mining algeritikeen

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https://sites.google.com/view/rampvis/

Model-specific visualizations 2.00 29%

Requirements

- Reproducible
- Traceable
- Validated
- Open source
- Open data

Open Epidemiology

https://github.com/ScottishCovidResponse

GITHUB ISSUES HPC THREADING

Administration

Lynn Esson (Glasgow) and Yasmin Abdalla (Edinburgh)

Rachel O'Brien (Glasgow) Mark Meenan (Glasgow)

Requirements

- Extreme patience

https://github.com/ScottishCovidResponse

Universities of Glasgow, Edinburgh, SRUC, Sheffield, Manchester, St Andrews, Stirling, Strathclyde, Heriot-Watt, Southampton, Cambridge, Oxford, Swansea, Bangor, Nottingham, Middlesex, City, U. of London, Warwick, Chester, King's College London, Loughborough, EPIC, Biomathematics and Statistics Scotland, UK Atomic Energy Authority, Met Office, Software Sustainability Institute, Man Group, Invenia, Horus Security, Red Sift Ltd, and others