Improving speed of models for improved real-world decision-making

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Abstract. In 2020, the rapid expansion of the COVID-19 global health crises meant that the speed of model development and analysis was critical to ensuring the right results were placed in decision-makers' hands as quickly as possible. For researchers in computational social science who may operate outside computer science faculties, making the leap between models built in platforms such as Netlogo and deployed on individual workstations vs high-performance computing (HPC) clusters can be great. Here, we present a set of generic templates that can be used and adapted by computational social science researchers who have access to HPC clusters but require additional support for deploying their models on this infrastructure. We show the improvements in model speed that can be gained through this process and discuss the practical importance of improving model speed for policy and decision-making in the real world.

1 Background

Computational social science is the discipline of representing communities, societies and social phenomena through the generation of tangible, observable, but computer-generated artificial or 'synthetic' societies. By authentically representing critical structures and patterns of interaction among agents within artificial societies, phenomena representing realistic potential crises befalling a society can also be generated[1]. Similarly, if crises within artificial societies can be generated, so too can policies that prevent those same crises from arising, as can potential solutions to crises that are unfolding or have already occurred.

The present gap between evidence that can be gathered from the construction, observation and analysis of artificial societies and the incorporation of this evidence into public policymaking primarily relate to bottlenecks in development, analysis and feedback. Very simply, the current time it takes to develop, analyse, and iterate trusted models of artificial societies is often too long to make them useful to policymakers. This delay can result in either 1) disengagement by time-poor policymakers who require faster answers to 'what-if?' questions than is

currently possible, or 2) the real-world crisis moves on to a new phase that is outside the scope of the current model. In both cases, the science has failed to keep pace.

There is urgent need for science and policy to connect better when faced with novel crises (e.g., COVID-19) requiring up-to date information and fast decision-making. Science needs to provide leaders, policymakers, and societies with clear, rapidly developed evidence delivered in as close to real-time as possible, and in a form that directly addresses policymakers' requirements[2]. High performance computing clusters are central to achieving this goal.

In this paper, we demonstrate the advantages for policy-making and analysis of deploying existing health-system policy models developed in Netlogo[3] on high-performance computing (HPC) clusters featuring parallel computing infrastructure. We provide a set of adaptable, step-by-step instructions and scripts that can be used as-is or modified with the assistance of local expertise to suit researchers' own HPC environments.

2   Method

To test improvement in speed associated with the deployment of policy-models on HPC clusters, we selected a model developed in consultation with the Victorian Department of Health and Human Services in Victoria, Australia to estimate risk associated with easing social restrictions after that state's 2nd wave of SARS-CoV-2 infections in 2020[4-6].

For simplicity, we compared a single scenario of 100 model runs under Policy 4 (aggressive elimination) from the published model. The count of model runs was controlled through the initialisation of 100 separate random seeds written into Netlogo's[3] BehaviourSpace function rather than by using the 'repetitions' function. We ran the model for a total of 1500 time-steps, equivalent to 1500 model days.

The model was first run on the author's laptop (Intel® Core™ i7-7700HQ CPU @ 2.80GHz, 32GB RAM, Windows 10, 64bit OS). It was then deployed using the 'Snowy' HPC partition on the University of Melbourne's 'Spartan' HPC cluster[7]. This is a traditional cluster with a high-speed interconnect in one partition as well as an alternative queue that uses virtual machines with a common image. Computing jobs are submitted to a Slurm workload manager specifying which par-

tition they would like to operate on (e.g., in our case, 'Snowy'). A contains detailed, step by step information on how to prepare existing Netlogo models for deployment on the HPC is contained at (insert Github location), however a brief outline follows.

Firstly, Netlogo must be installed to run on the HPC cluster. Next a Netlogo model must be created to match the format required for deployment. Any Netlogo dependencies and plug-in packages (e.g., rngs, GIS, etc.) copied to the same folder to the Netlogo model.

Regardless of the type of model, it must contain a named experiment within the BehaviourSpace function that contains a number of random seeds equal to the number of individual runs desired for each unique parameter combination. For example, 100 random seeds, combined with 3 policy setting choices on (example) variable 1 and 5 choices on (example) variable 2 would result in 100 x 3 x 5 = 1500 individual model runs containing 100 runs of 15 separate policy combinations.

Using the set of templates found at (inset repository), the user can open the 'Revise and Run all in one.sh' file, altering the highlighted inputs to match the Netlogo file location, the unique BehaviourSpace model name, and the desired output file name location. Running this file in the command line will create a folder containing 100 separate .xml files which will be submitted as independent jobs across the HPC cluster and contain the full complement of parameter combinations.

Next, the experimenter can open and revise the 'submit_jobarray.slurm' file, again altering details related to file locations, input and output folders, as well as SBATCH settings unique to their own HPC environment. In our example we set the number of nodes per job, the desired partition on the HPC, the job name, the maximum run time for any job, and the desired CPUs per task (8). The HPC cluster at Unimelb also allows priority for COVID-19 research jobs, enabling them to skip the queue for deployment.

3   Results

Run-time for the model deployed over 100 runs on the researchers' laptop was 2 hours, 26 minutes. By comparison, CPU time for the same model deployed on the HPC was 37 minutes, 36 seconds, while job wall-clock time was 4 minutes, 14 seconds. Deploying on the HPC cluster resulted in a 34x increase in real-time speed.

4   Discussion

A hindrance to the uptake of computational social science and synthetic societies research programs to date has been the speed at which models can be developed and at which results of synthetic policies can be trialed, analysed and fed back to policymakers. This was highlighted in the early stages of the COVID-19 pandemic where highly influential models in both the UK and Australia were adapted from existing representations of influenza spread rather than built as bespoke representations[8]. It shows that in urgent crises where answers are demanded in hours rather than months, the capacity to ramp-up model speed and analysis is critical.

In our own work with the Victorian Government during the second wave COVID-19 crisis[6, 9], extreme time pressure was exerted to match the timeframe of Victorian 'Crisis Cabinet' deliberations, resulting in advice being omitted if deadlines were not met. This situation motivated us to build and share these templates for adaptation and use by other researchers lest the value of insights provided by our work be neglected simply on the basis of that advice being too slow to generate.

Our discipline's models must of course be robust, but it is also important to recognise that sometimes policy and decision-makers cannot wait for the completion of our work. Important decisions will be made regardless [10]. The speed at which models and synthetic evidence can be produced has the potential to significantly affect the course of strategy, policy direction, action and public health in urgent crises.

References

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