



australian partnership for
advanced computing



GIN Interoperability DEMO

SC07

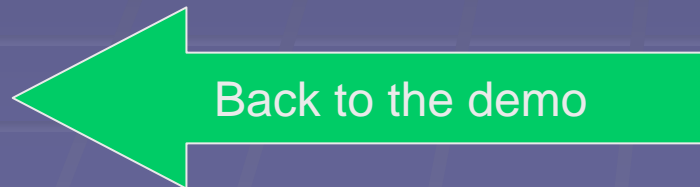
Kenton D'Mellow
Michael Rambadt
Andrea Vanni

Scientific background

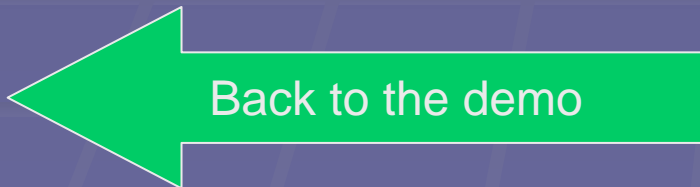
- HIV is a disease that effects some 40 million people worldwide
- Certain drugs can improve patient health by binding to and inhibiting critical viral enzymes
- Virun can mutate and become resistant to these drugs
- This simulation is designed to gather drug binding interaction energies of anti-HIV drugs bound to the active site of HIV protease, including drug-resistant versions of the protein.

Scientific background

- DRUG BINDING AFFINITIES OF HIV DRUG RESISTANT STRAINS
- The aim of this demonstration is to provide a range of simulations of known mutants against one particular HIV drug, Aprenavir.

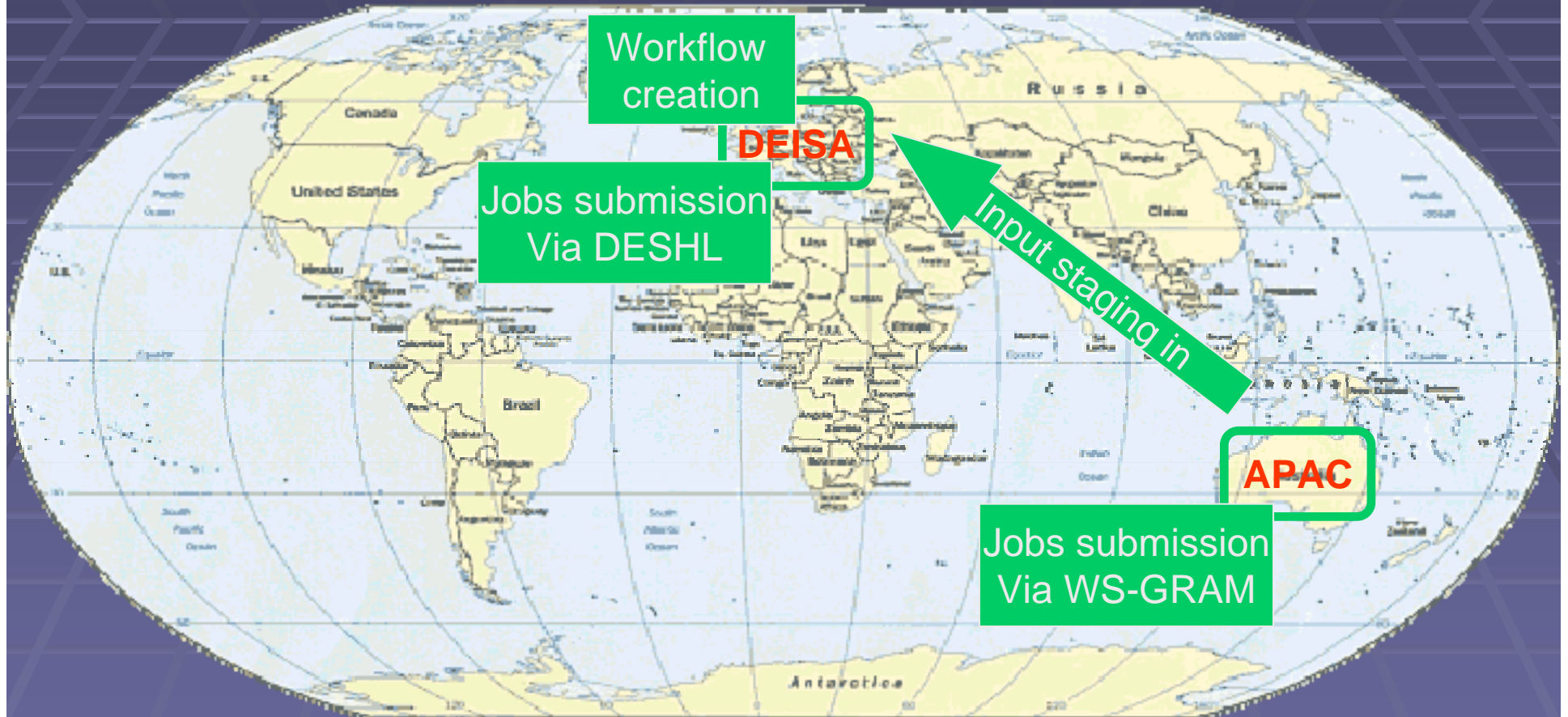


Computing resources background



Demo workflow

workflow creation and input file staging in



Workflow creation

DEISA

Jobs submission
Via DESHL

Input staging in

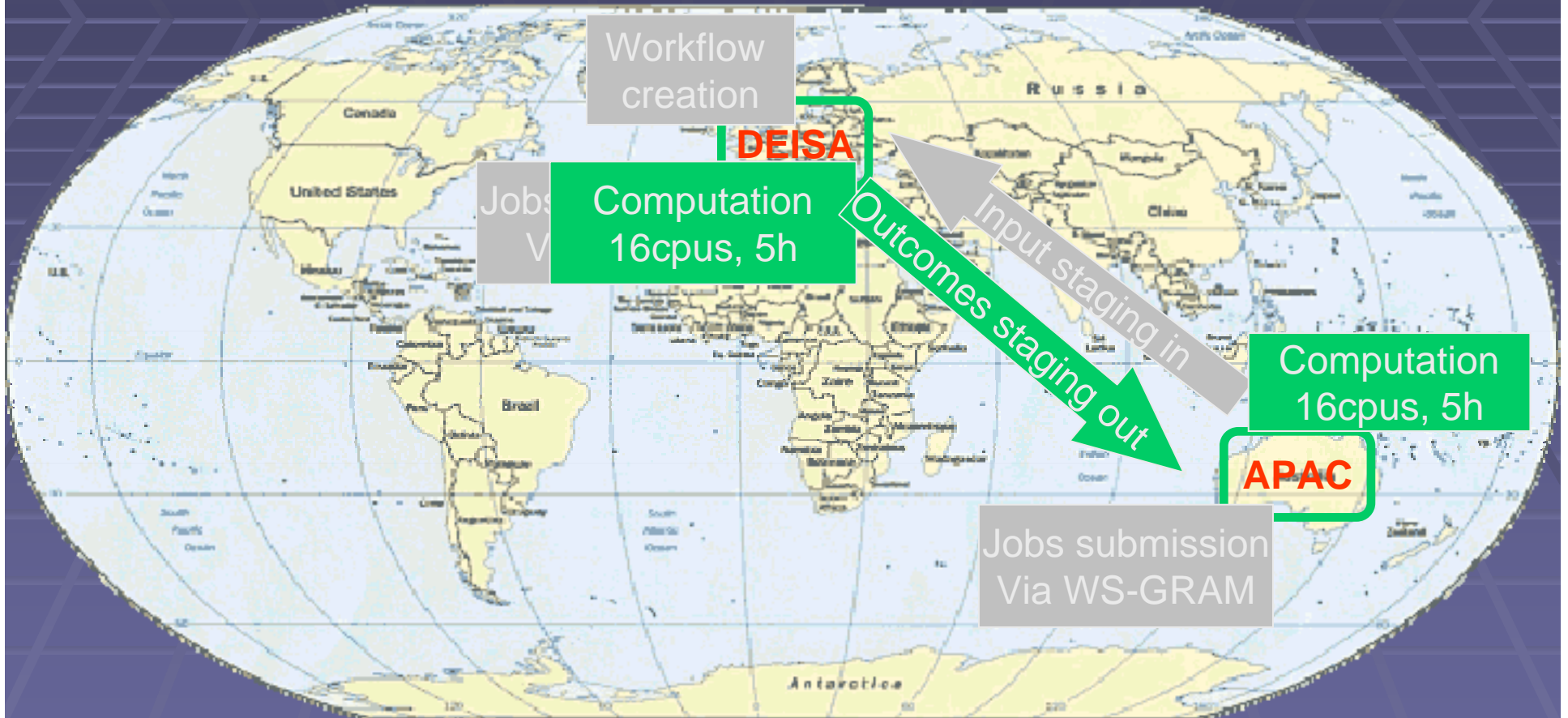
APAC

Jobs submission
Via WS-GRAM

Back to the demo

Demo workflow

Monitoring & staging out



Back to the demo

Demo workflow post-processing

