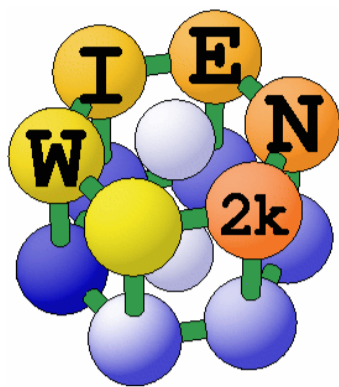
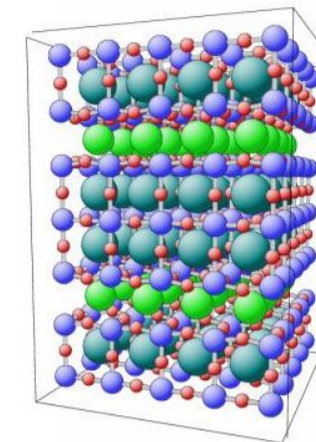


# ASKALON

Real World Workflow Applications  
in the Askalon Grid Environment



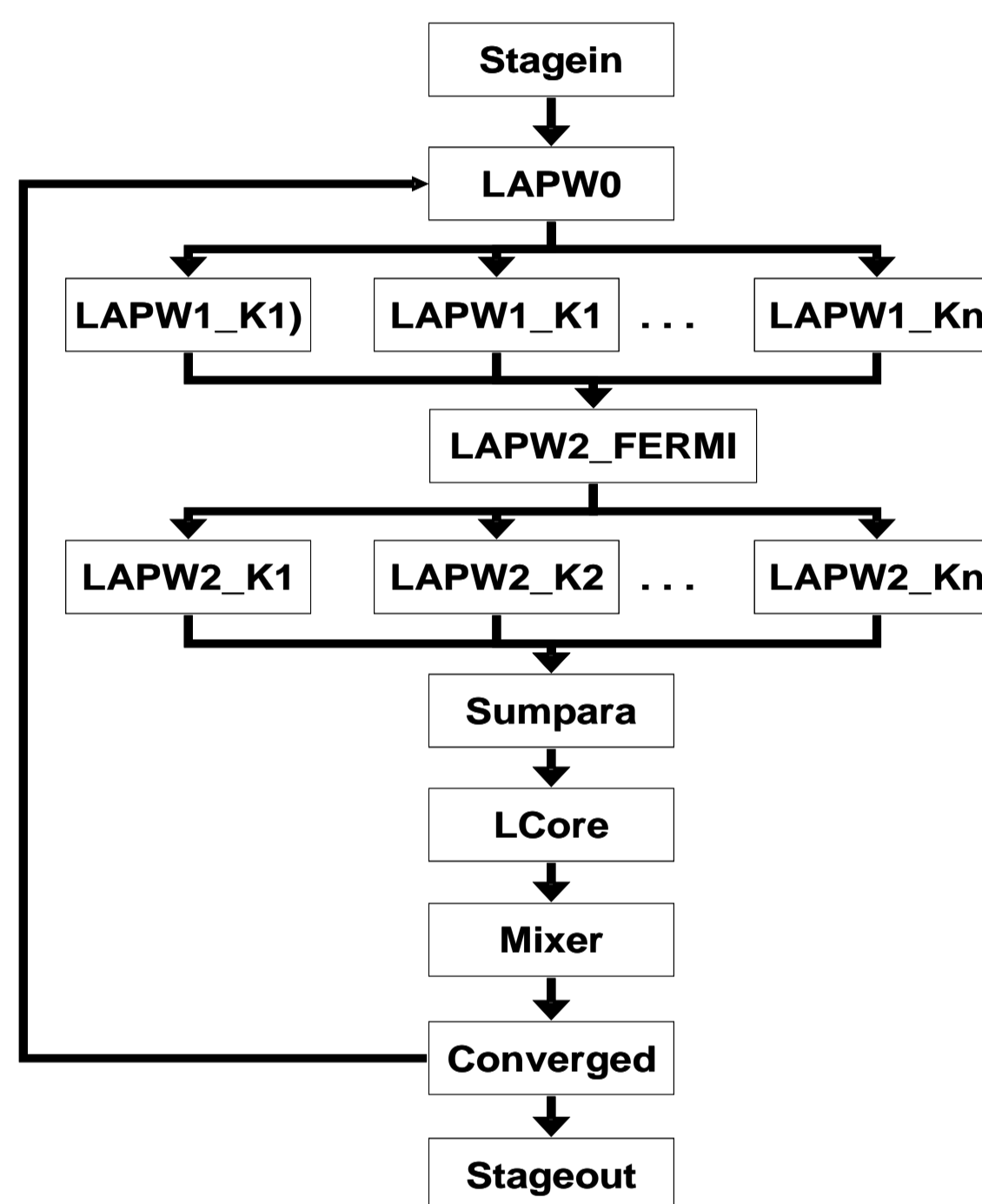
## WIEN2k



WIEN2k is a program package for calculating the electronic structure of solids based on the Density Functional Theory and the Augmented Plane Wave method. The WIEN package is being developed at the Institute for Material Chemistry, Vienna University of Technology, Austria, since over 20 years and has been licensed world-wide by more than 750 groups in academia and industry.

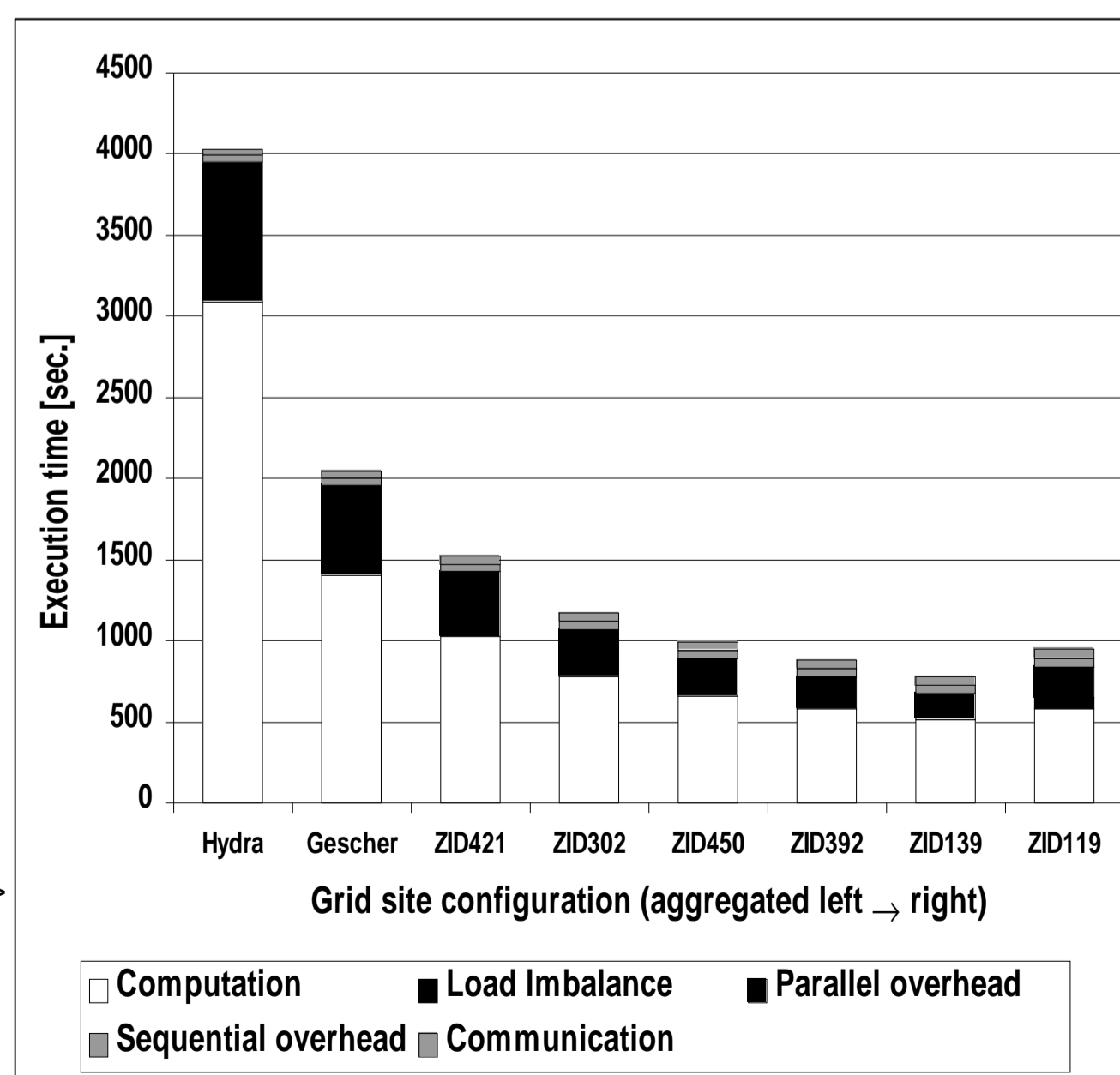
### WIEN2k Grid Workflow

Grid workflow applications are specified in ASKALON at a high level of abstraction using the UML-based modelling tool Teuta or the XML-based **Abstract Grid Workflow Language (AGWL)** that shield the user from the low-level Grid implementation technologies. Teuta and AGWL support scalable **parallel loop** constructs to express large activity parallelism in the WIEN2k workflow. The workflow is automatically translated to a **concrete representation** bound to Fortran legacy applications executed on the real Grid using the ASKALON middleware (meta-scheduler, execution control and resource broker). ASKALON employs a **genetic search scheduling algorithm** to find optimal mappings of the workflow activities onto the computational Grid resources. By incorporating the ASKALON environment, we could dramatically **improve the execution time** of a large WIEN2k problem size on the Austrian Grid. For instance, by using only 7 Austrian Grid sites which aggregate over 250 heterogeneous processors, we achieved a performance improvement of a factor of six compared to the fastest parallel machine available in this Grid infrastructure.



```

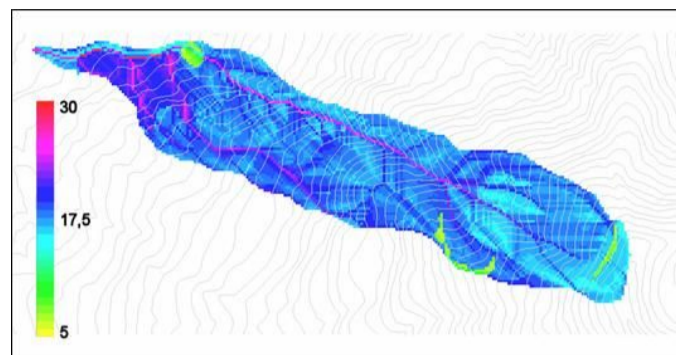
<agwl>
<importATD url="http://..." prefix="w2kAtd"/>
<workflow name="wfWien2k">
<dataIn name="fileIn0" source="tic.in0"/>
<body> <sequence>
<while name="whileTestConv">
...
<condition> val='true' </condition>
<loopBody>
...
<parallelFor name="pforLAPW1">
<dataIn name="fVsp" source="outFileVsp"/>
...
<loopCounter name="i" from="0" to="n"/>
<loopBody> <sequence>
<activity name="LAPW1" type="...">
</activity>
</sequence> </loopBody>
</loopBody> </while>
<dataOut name="outVal" source="val"/>
</while> </sequence> </body>
<dataOut name="outVal" source="..." saveTo="..." />
</workflow>
</agwl>
  
```



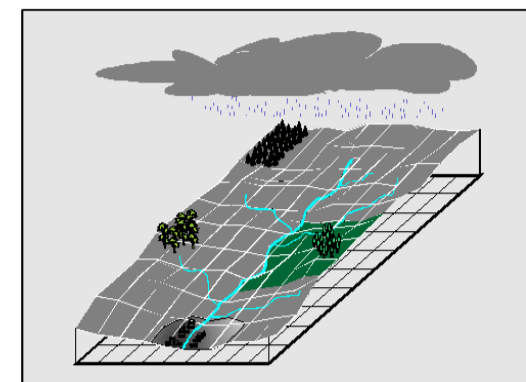


# ASKALON

Real World Workflow Applications  
in the Askalon Grid Environment



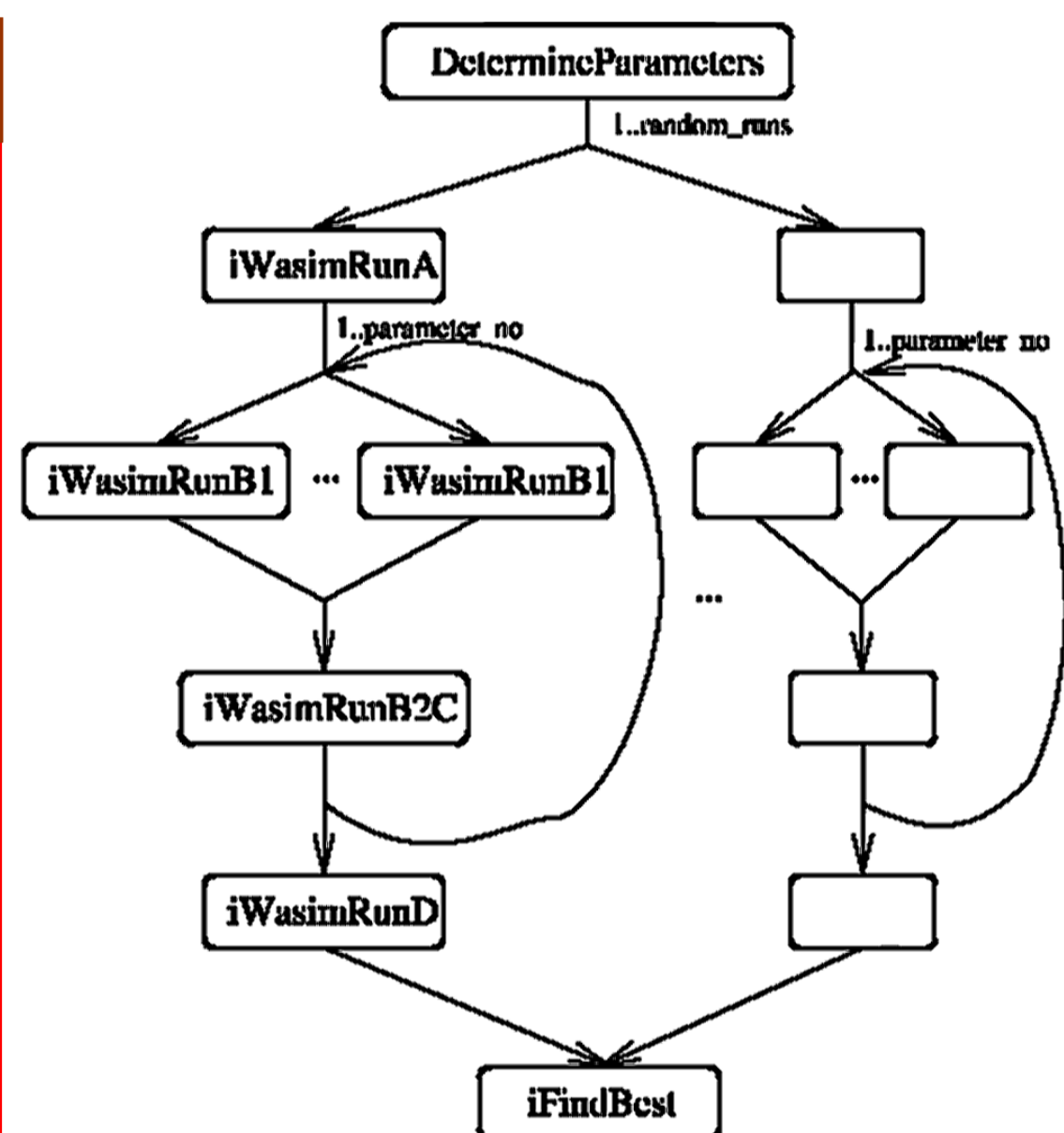
## Invmod



Invmod is a program package developed at the Institute of Hydraulic Engineering, University of Innsbruck, Austria, that combines new measurement technologies with numerical computations to obtain improved discharge estimates for extreme floods. Invmod employs the widely used WaSim hydrological program developed at the Swiss Federal Institute of Technology to conduct the simulations.

### Invmod Grid Workflow

Grid workflow applications are specified in ASKALON at a high level of abstraction using the UML-based modelling tool Teuta or the XML-based **Abstract Grid Workflow Language (AGWL)** that shield the user from the low-level Grid implementation technologies. Teuta and AGWL support scalable **parallel loop** constructs to express large activity parallelism in the Invmod workflow. The workflow is automatically translated to a **concrete representation** bound to Fortran legacy applications executed on the real Grid using the Askalon middleware. ASKALON employs a **genetic search scheduling algorithm** to find optimal mappings of the workflow activities onto the computational Grid resources. We have **improved the execution time** of several large Invmod problem sizes by a factor of four compared to the fastest parallel machine available by **distributing the workflow onto seven sites of the Austrian Grid**, which aggregates over 250 heterogeneous processors.



```

<agwl>
<importATD url="http://..." prefix="invAtd"/>
<workflow name="wfInvModG">
  <dataIn name="invModGIFile" source="..."/>
  <body> ...
  <while name="while1">
    ...
    <condition>repeatLoop='true'</condition>
    <loopBody>
      <sequence name="seq3">
        <parallelFor name="pfor2">
          <dataIn name="noOfParams" source="..."/>
          <loopCounter name="j" from="0" to="n"/>
          <loopBody>... </loopBody>
          <dataOut name="wB10Files" source="..."/>
        </parallelFor>
        ...
      </sequence>
    </loopBody>
  </while>
  ...
</body>
<dataOut name="res" source="..." saveTo="..."/>
</workflow>
</agwl>
  
```

