Practical Experience from Porting the Wien2k Application to EGEE

Max Berger
University of Innsbruck, DPS
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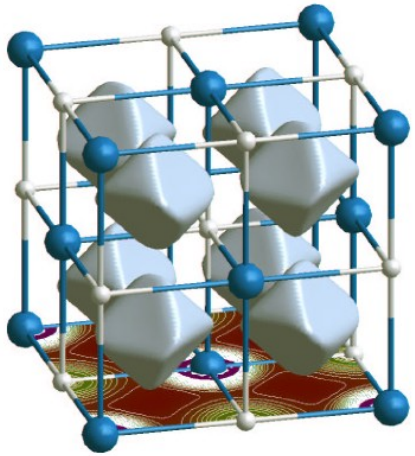
Information Society

Outline

- **Introduction**
  - Wien2k
  - Grid Workflow
  - Grid Scheduling
- **Evolution of Workflow execution**
  - Naïve
  - Worker model
  - Re-use deployment
  - Smarter data Transfer
  - SE Data Transfer
  - P2P Data Transfer
- **Conclusions**

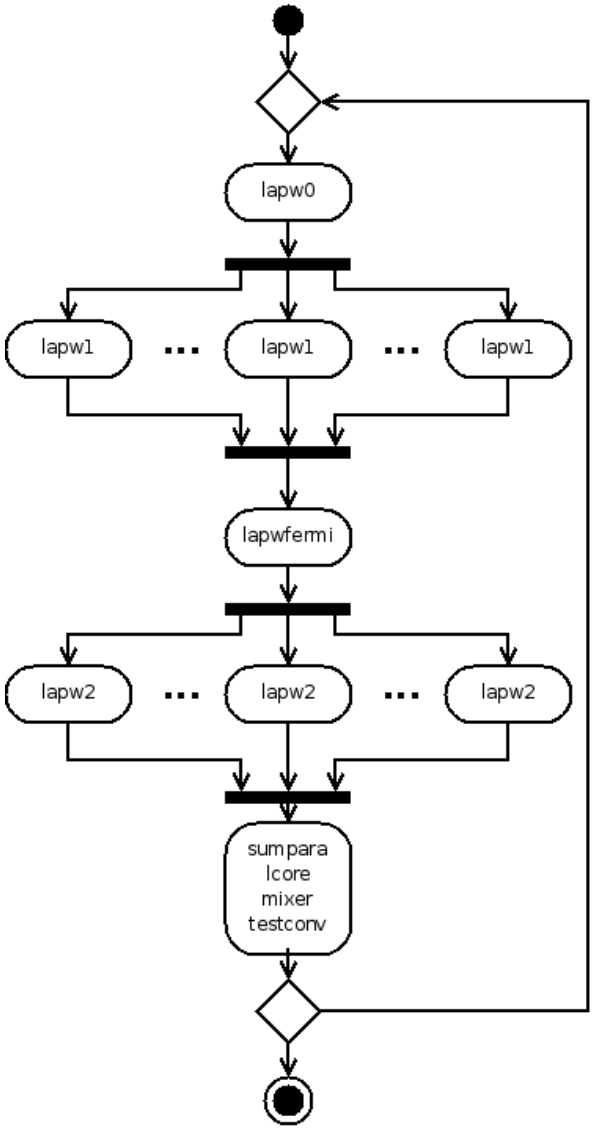
Wien2k

- Performs electronic structure calculation of solids (crystals)
- Based on full-potential (linearized) augmented plane-wave ((L)APW) method
- One of the most accurate schemes for band structure calculations
- Developed by Computational Quantum Chemistry Group at Tech. Uni. of Vienna (K. Schwarz, P. Blaha)
- Over 1000 licenses world-wide
- Sequential and MPI versions



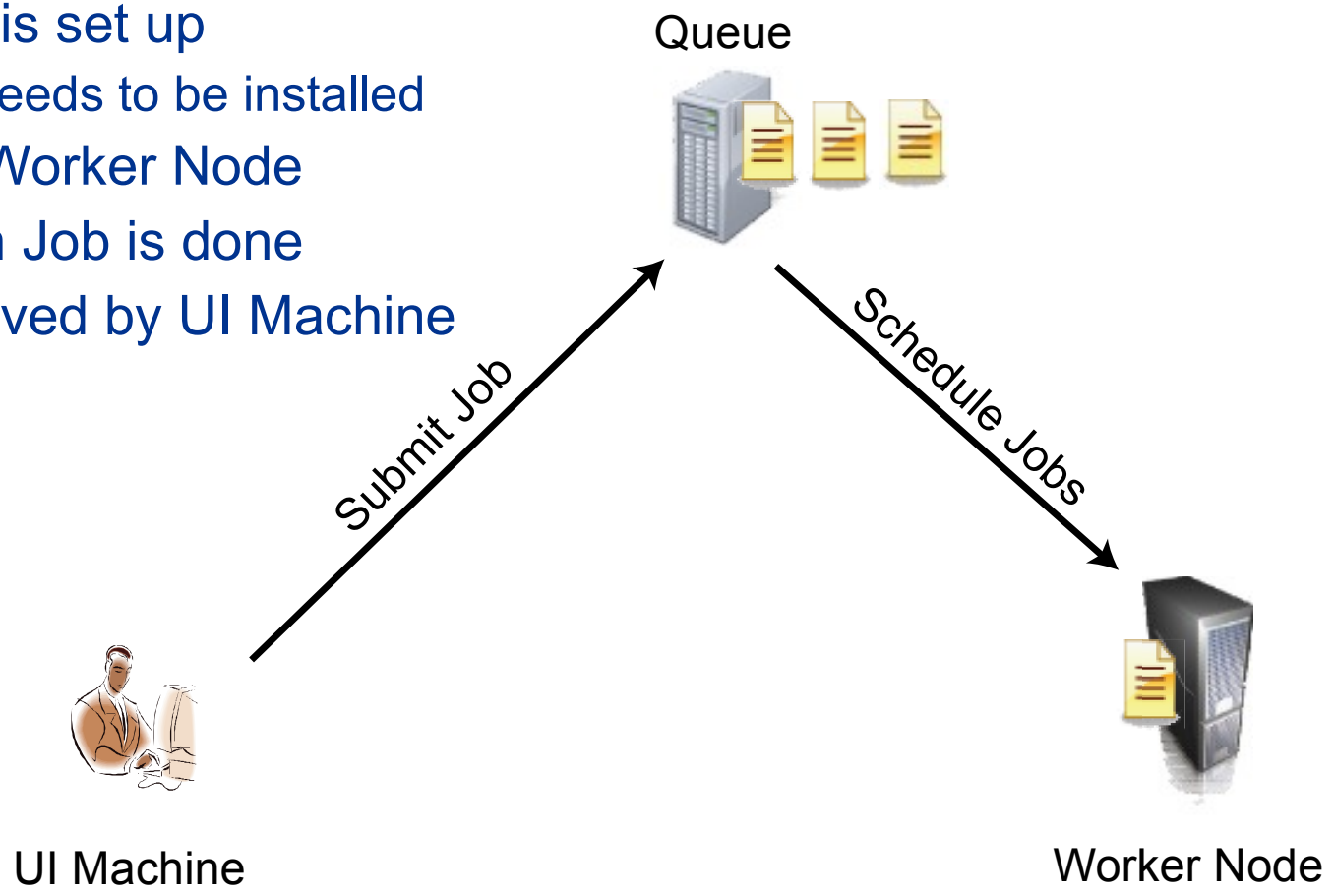
Grid Workflow

- **Focus on SCF-Cycle**
- **Identify atomic and compound activities**
  - Atomic: single activities
  - Compound: Can be splitted and parallelized
- **Application activity ≠ Grid activity !**
- **Grid activity**
  - wraps application activity (or activities)
  - can run independently of the others
  - performs data flow management
  - sets environment
  - cleanup environment



Grid Scheduling

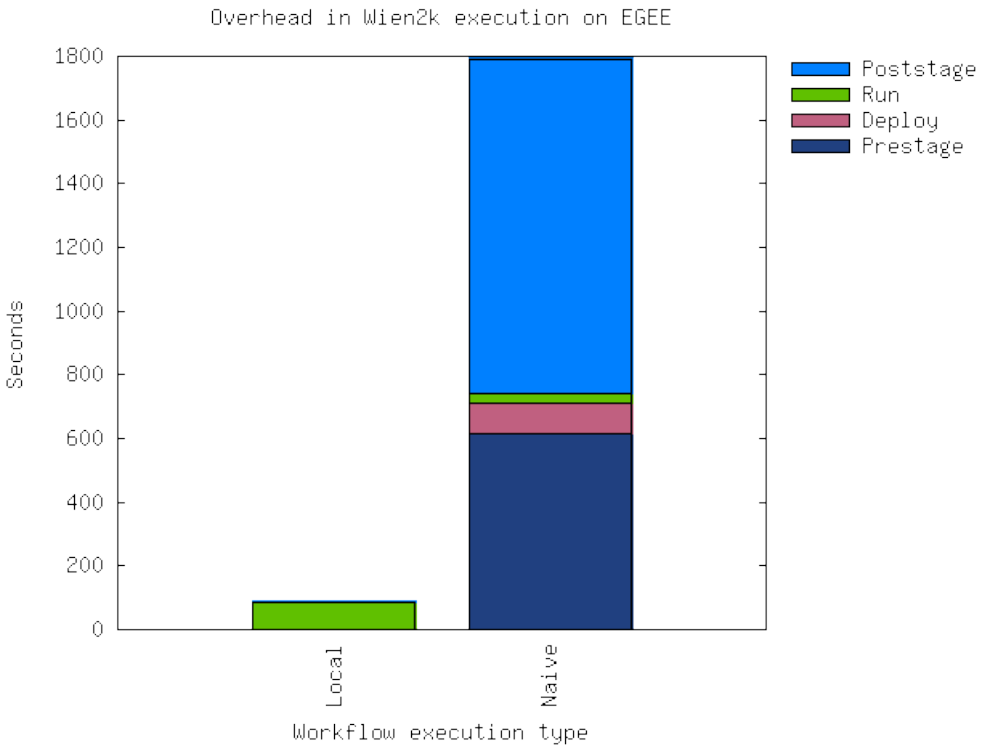
- **Scheduling Latencies**
  - Grid Job → Job Que
    - EGEE: WMS Que + Site Que
  - Environment is set up
    - Software needs to be installed
  - Job runs on Worker Node
  - Notifies when Job is done
  - Results retrieved by UI Machine



Evolution of Workflow Evolution

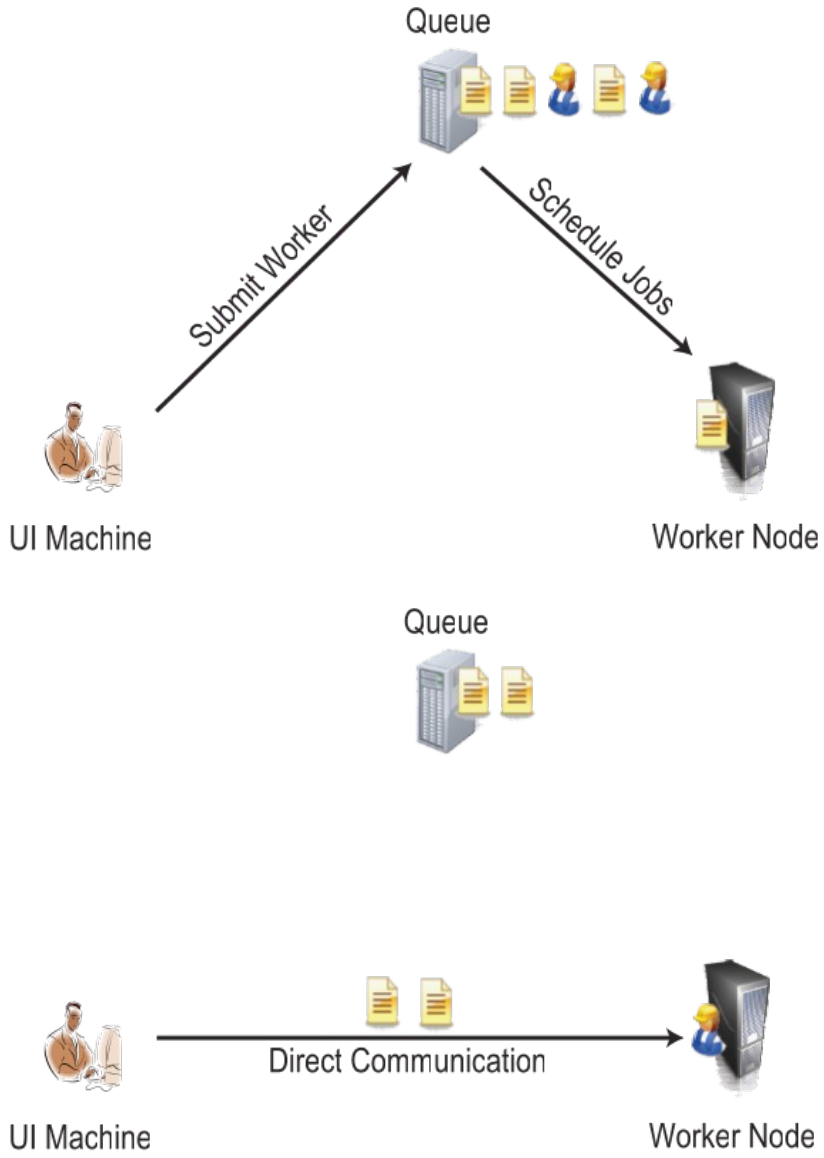
Naïve Scheduling

- **Each Activity is mapped to One Grid Job**
- **Works well in research Grids**
- **Does not work in Production Grid (EGEE)**
  - Scheduling Latency mean: 121 seconds!
  - Done → Done notification: 208 seconds!
- **Too much overhead!**
  - Works only with large workloads



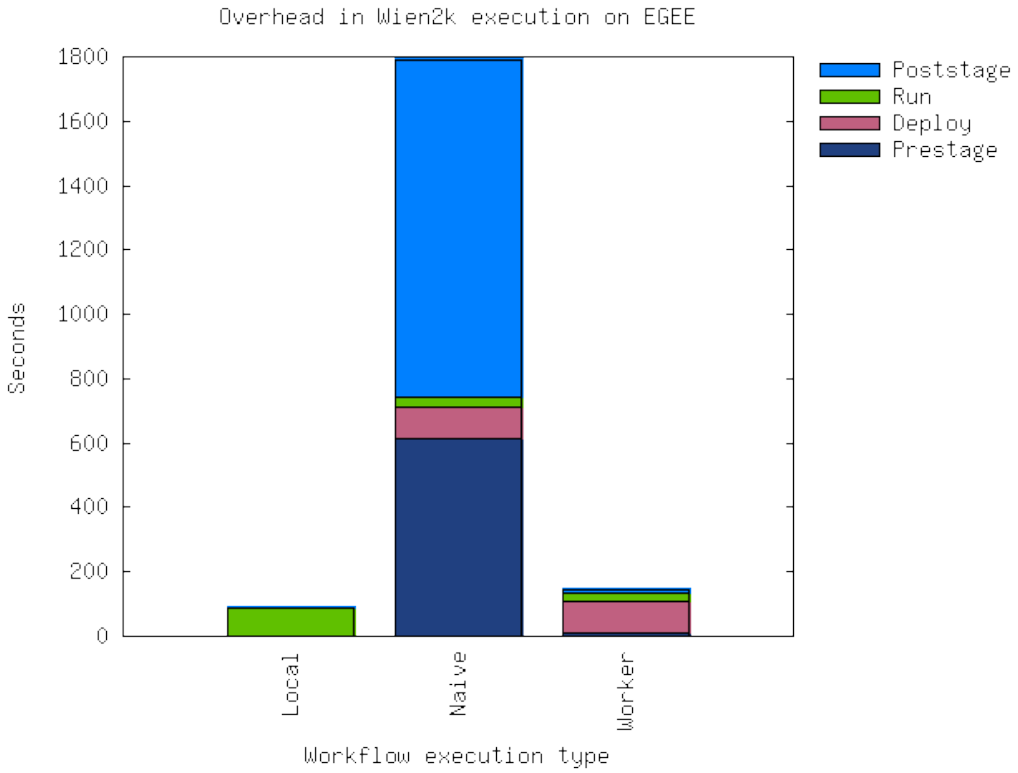
Worker Model

- **Worker Model**
  - Submit workers instead of activities
  - Submission Que is used only once
  - Workers pull from master
- **Used by**
  - Ganga (called Pilot Model)
  - Many other WF engines
- **Issues**
  - May be unfair



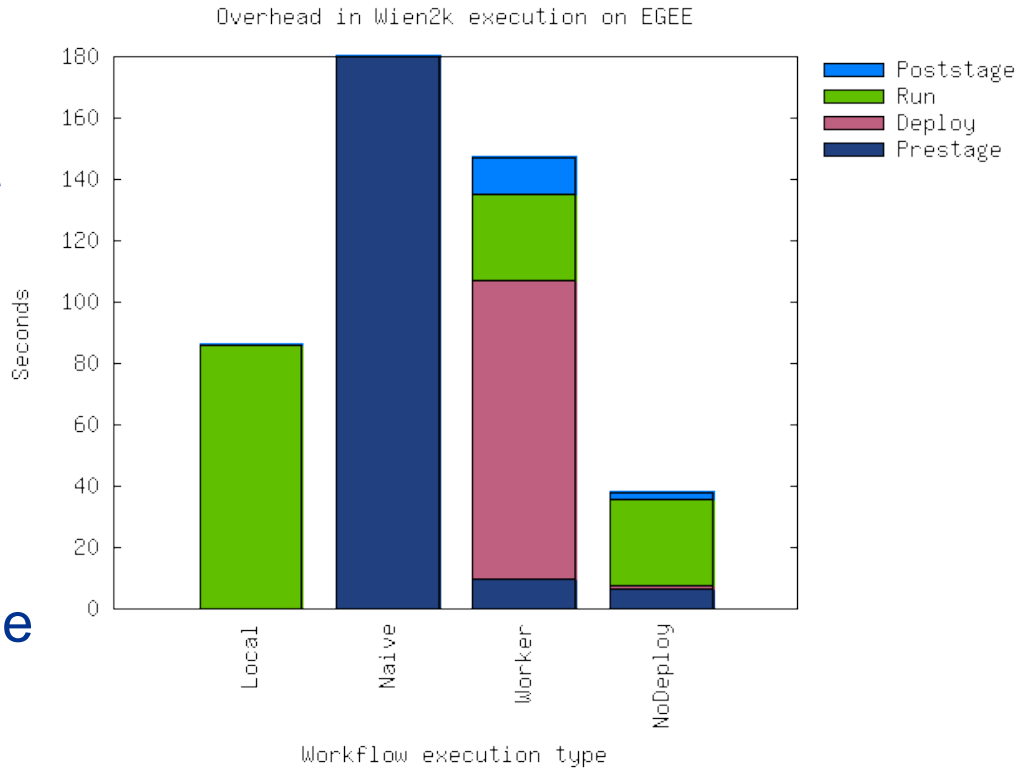
Worker Model (cont.)

- Brings execution time down to feasible range
- Good for medium sized problems
- More optimization possible



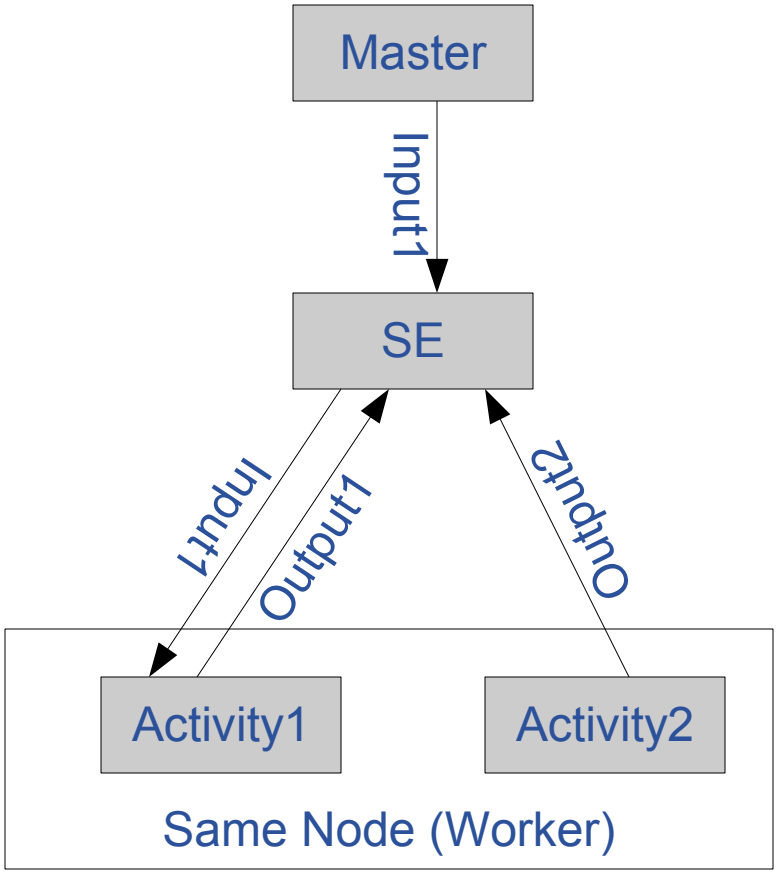
Re-use deployment

- **Wien2k Software is proprietary software**
  - No permanent deployment
  - Automatically deployed before execution
  - Deleted after execution
- **Worker advantages**
  - Deploy once
  - Delete once the WF is done



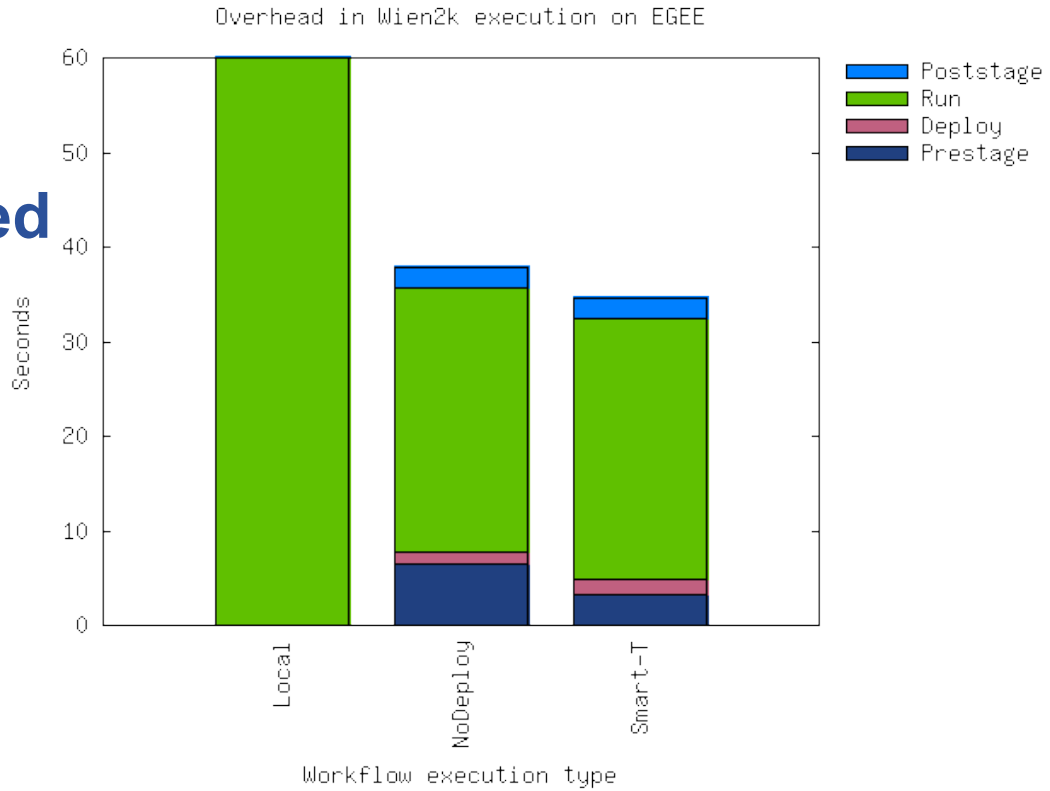
Smart Data Transfer

- **The Worker stays on a Grid node**
  - It can reuse data from the last activity it performed
- **Keep list of active data**
- **Only transfer new files**
- **Common Caching problems**
  - File may be outdated
  - Still need to publish output



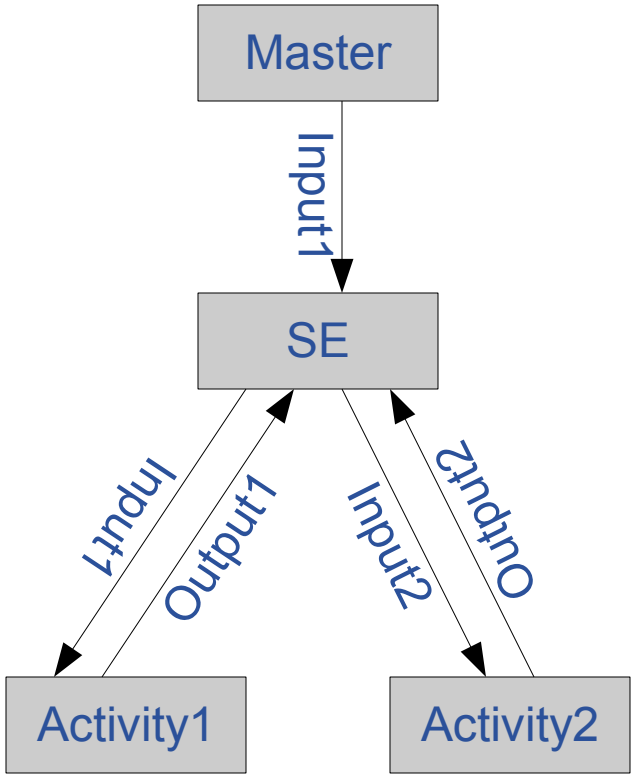
Smart Data Transfer (cont.)

- Upload time is shortened
- Good result
- Little overhead



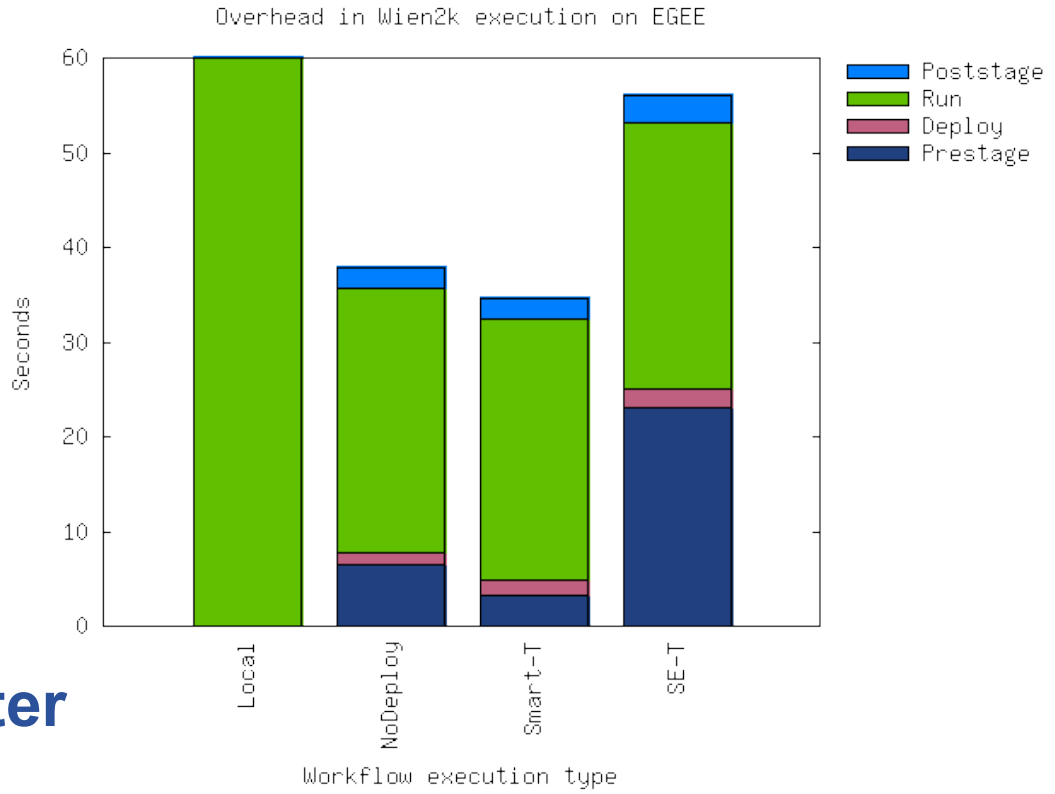
SE Data Transfer

- **Data is stored on the Master**
  - Data is submitted along with the activity
  - Results are published back to the master
- **Data is stored on a Storage Element (SE)**
  - Initial Data is uploaded to the SE
  - Activities publish to and pull from the SE



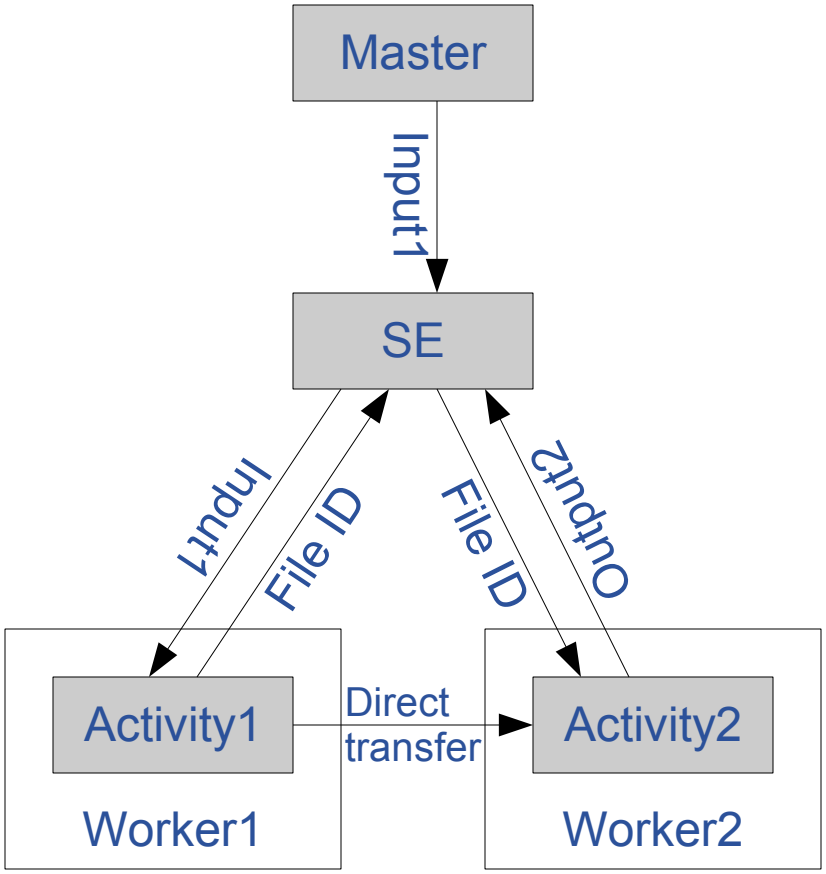
SE Data transfer (cont.)

- **SE Data transfer is slower than transfer from / to master!**
  - SE may be in different country
  - Master is also on wired network
- **Creation overhead**
  - LFC communication
  - SE communication
- **Only interesting if master is on a slow network**
  - Laptop at Conference



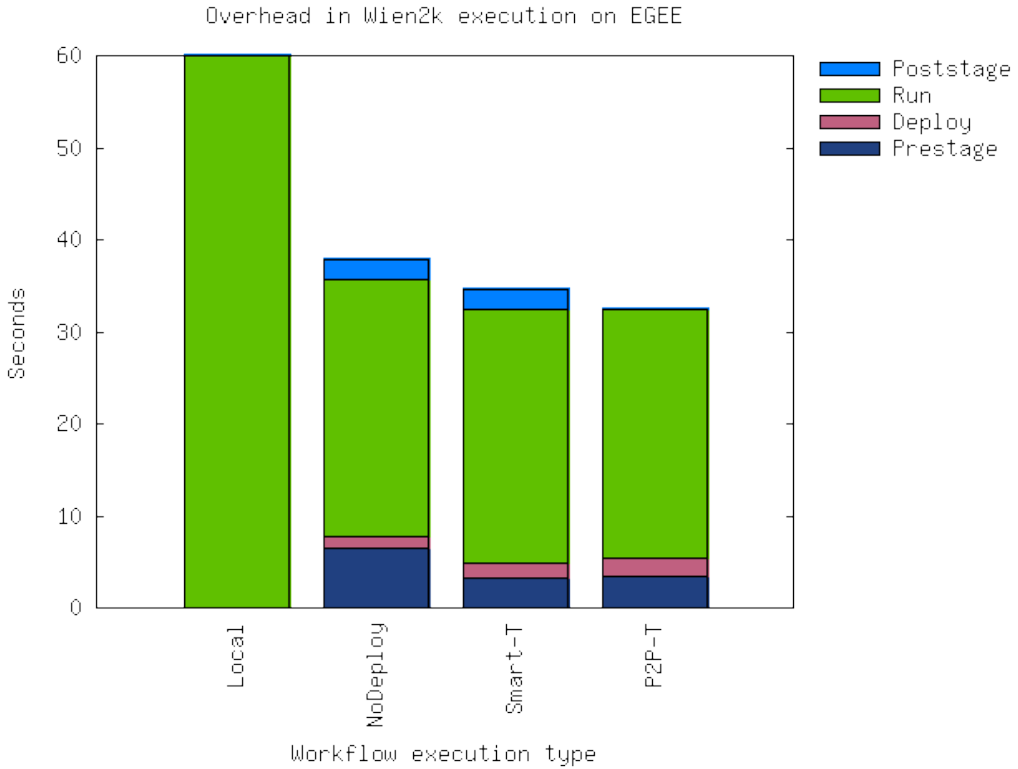
P2P Data Transfer

- **Activities on different workers?**
  - Files are transferred twice (to and from SE / Worker)
- **Use direct connection**
  - Save 50% Bandwidth!

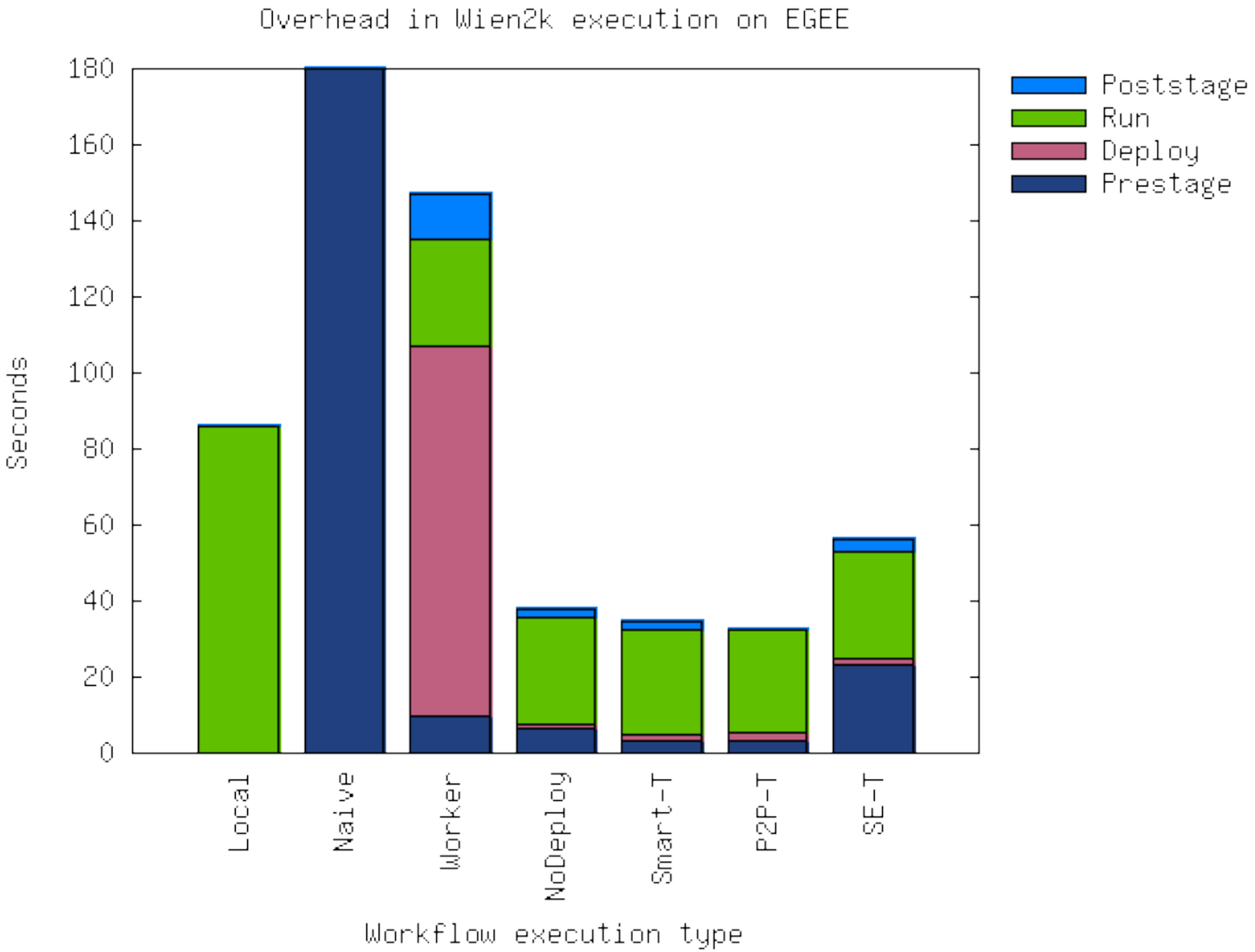


P2P Data Transfer (cont.)

- **Issues**
  - Reliability of workers
  - Firewalls
- **Connection overhead**
  - Not viable for small files
- **Management overhead**
- **Network is too fast!**
- **Results do not justify additional complexity**



Complete Results



Conclusions

- **The Wien2k applications runs well on the Grid**
  - Workflow is ported
  - Scheduling issues are solved
  - Data transfer optimization
- **The results can be applied to any application workflow**
- **Wien2k porting is finished**
- **Work on packaging for the end user**
- **Side effects:**
  - Yet another WF engine
  - Programming API for gLite which does NOT require a gLite UI