A priori modeling of chemical reactions on a grid-based virtual laboratory

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Outline

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Modeling chemistry

Simulating processes on a molecular basis

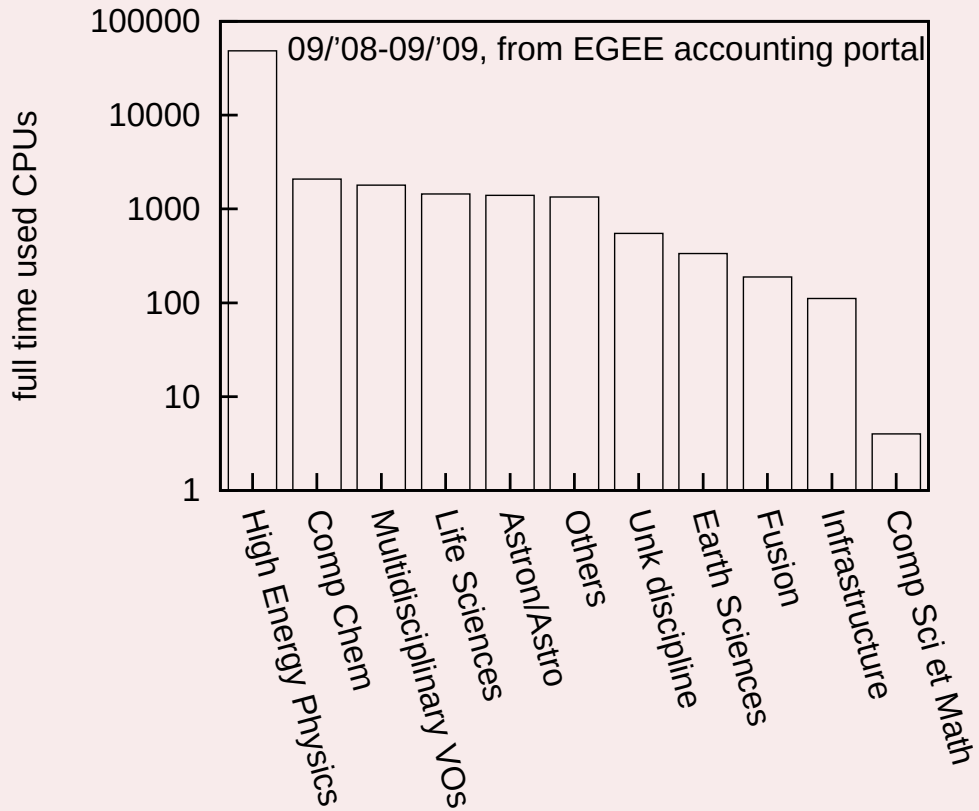
- modeling natural phenomena
- designing new materials
- mastering new technologies

. . . requires

- assembling various pieces of software
- converging different competences
- a world spread virtual laboratory

. . . on the Grid:

A self-introducing picture



The Grid Enabled Molecular Simulator

GEMS is

A grid based realistic simulator that can act as a molecular science engine in complex multiscale chemical contexts.

The recipe

- software: a suite of codes
- interoperability: standards and tools
- a director: workflow management
- a factory: Grid, the modern paradigm of HTC

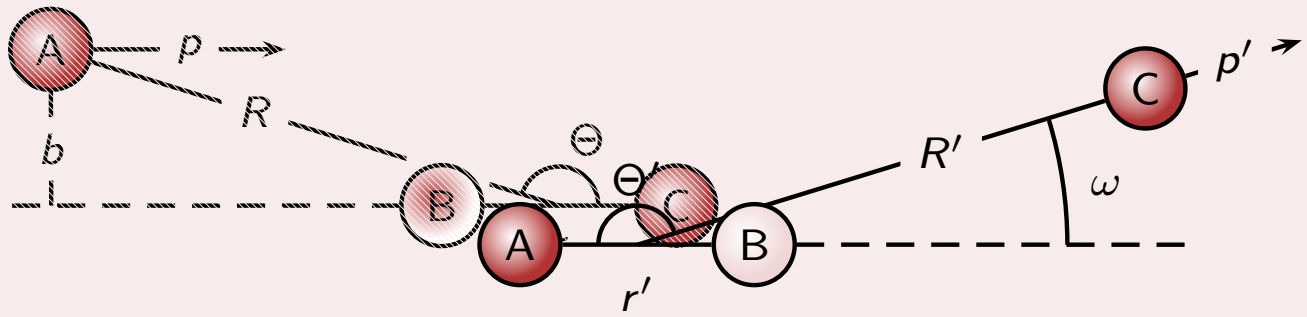
Let's start with a few atoms...

Outline

The quantum view

A reactive collision

$$A + BC\ (v,j) \rightarrow AB\ (v',j') + C$$



The B-O "equation of motion"

$$i\hbar\frac{\partial\psi(\mathbf{w},t)}{\partial t} = \left[\hat{T}_{\mathbf{w}} + V(\mathbf{w})\right]\psi(\mathbf{w},t)$$

Solution methods

If $\hat{H} \neq f(t)$, then either (TD methods)

$$\psi(\mathbf{w}, t+\tau) = e^{-\frac{i\hat{H}\tau}{\hbar}}\psi(\mathbf{w}, t)$$

Or simply (TI methods)

$$\hat{H}\psi(\mathbf{w}) = E\psi(\mathbf{w})$$

From an analysis on ψ

The detailed scattering matrix elements $S^J_{cv'j'k',avjk}(E)$

Quantities of interest

From the state to state **S** elements

- detailed reaction probabilities
- state to state differential cross sections
- integral cross sections

Further elaborating...

- branching ratios
- product internal energy distributions
- microscopic branching
- reaction rates

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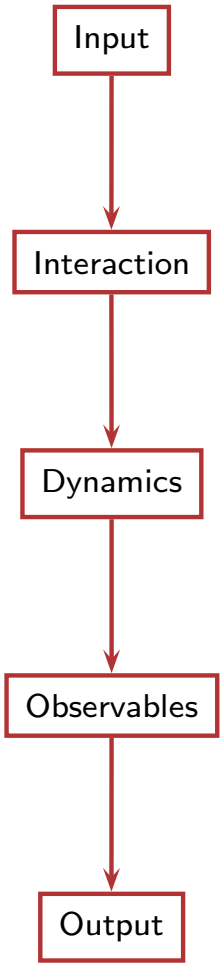
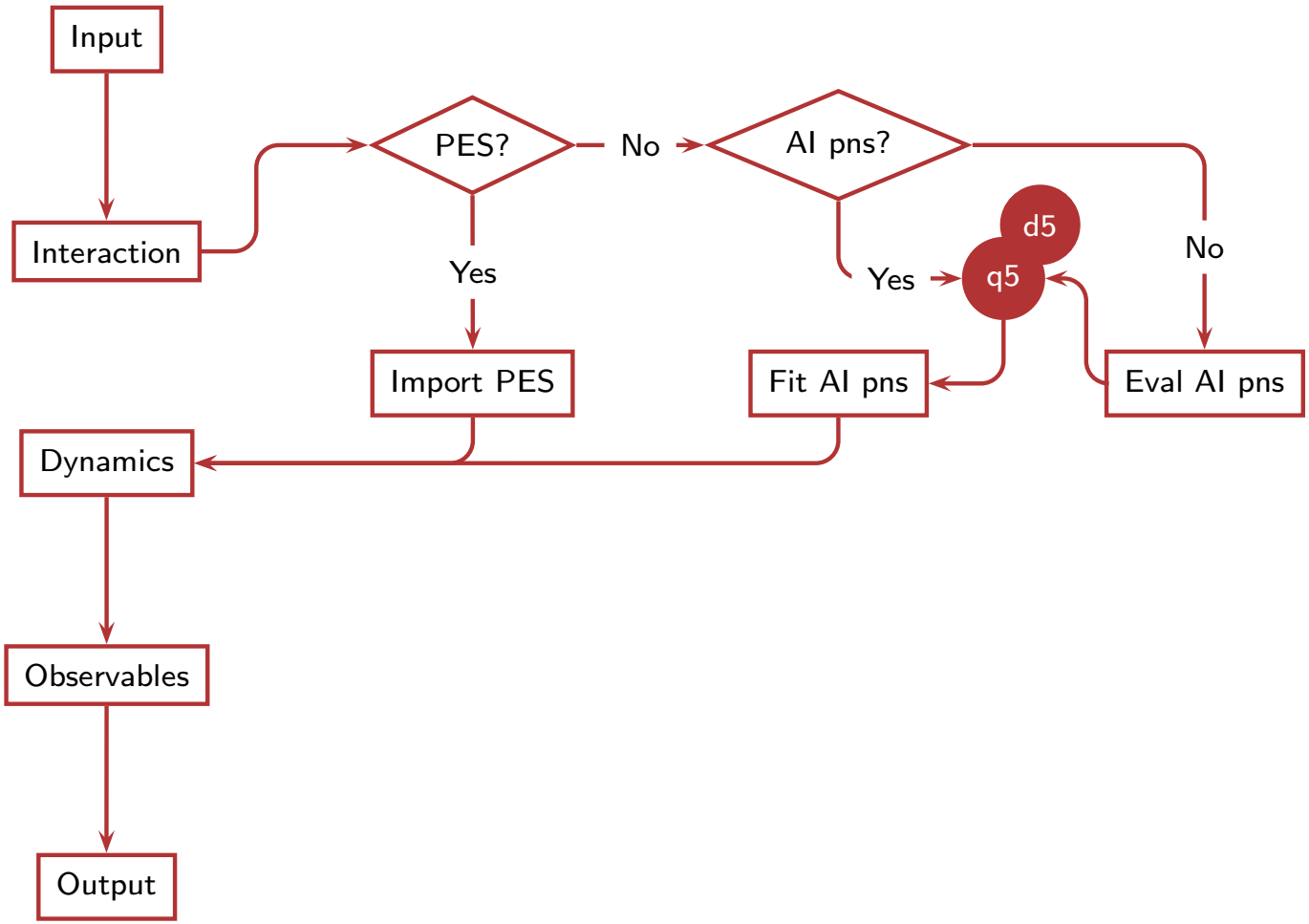
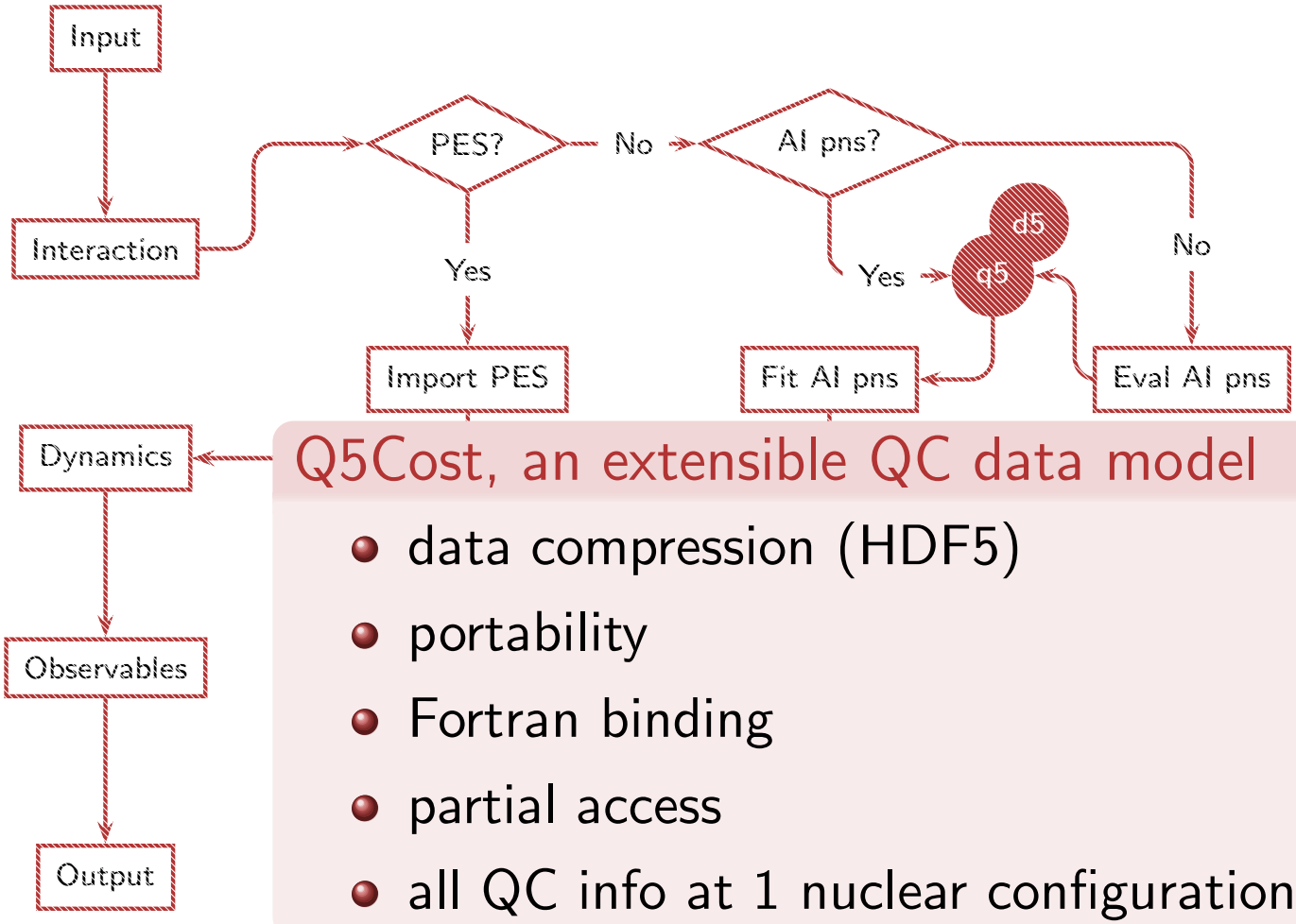
Overview



The Interaction module



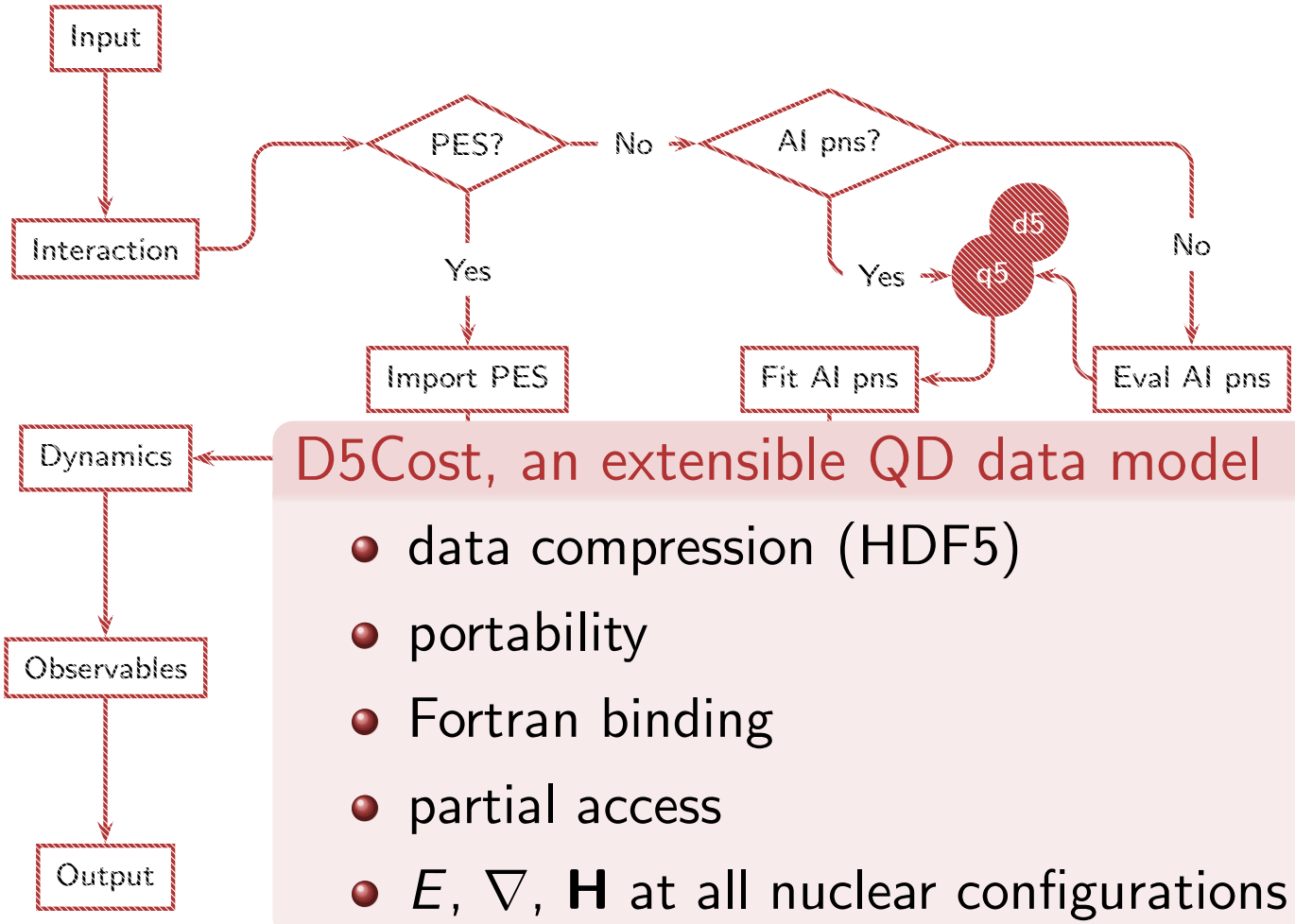
Interoperability in Quantum Chemistry



Q5Cost, an extensible QC data model

- data compression (HDF5)
- portability
- Fortran binding
- partial access
- all QC info at 1 nuclear configuration

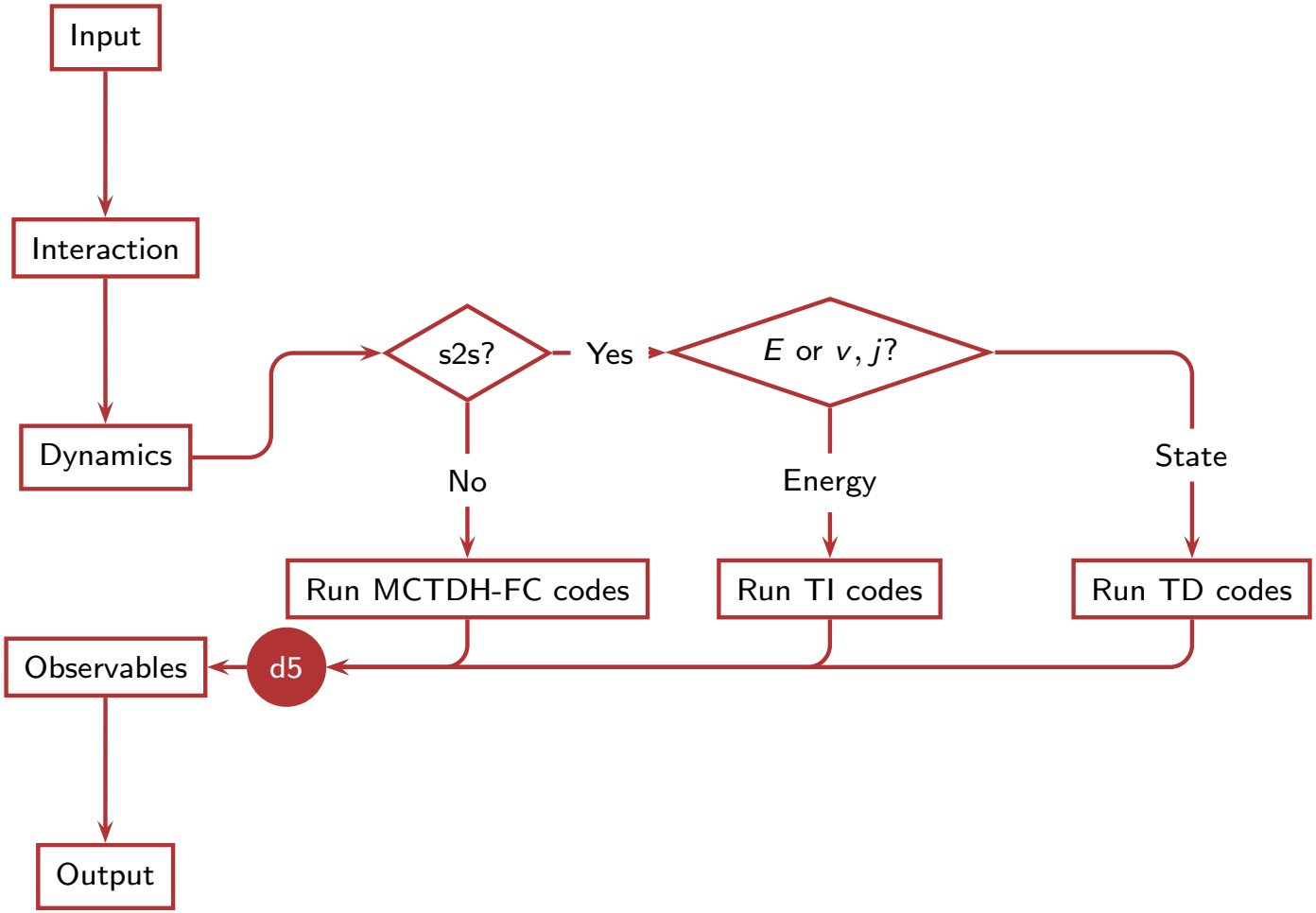
A bridge to Dynamics



D5Cost, an extensible QD data model

- data compression (HDF5)
- portability
- Fortran binding
- partial access
- E, ∇, $\mathbf{H}$ at all nuclear configurations

The Dynamics module



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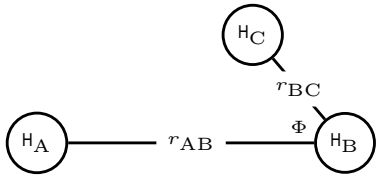
Computing details

$H + H_2\ (v,j) \rightarrow H_2\ (v',j') + H$

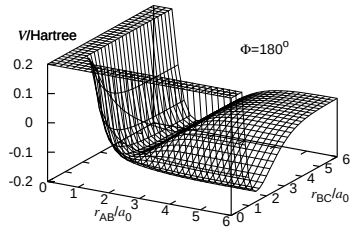
- `DALTON`: 269 H_3, 22 H_2 points
- `GFIT3C`: fit to a PES (.f)
- `ABC`: run 1000 null-J E's over

At present

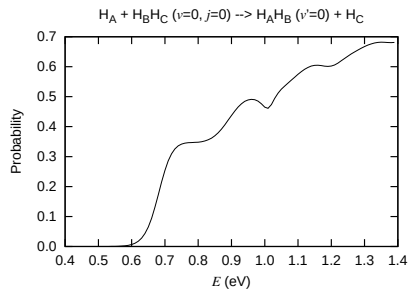
only ABC ported to EGEE



Distribute AI runs and get the PES



Distribute scattering E's and get reactive P's



ABC: a comment on the distribution

Execution time

almost linear with number of E's per run:

- 1000 E's 1 run, local machine: 21 m

Though,

the "Grid overhead" is umpredictable. . .

Grouping E's

a compromise between speedup and employed resources:

- 100 E's per run, 10 CEs, 2 casts: 4 m

Outline

Building GEMS...

Scientific software

port to the Grid, integrate in GEMS

Vertical interoperability

between classes of codes from different domains

Workflow management

a bash script, at present...

User friendly interface

buttons, menus, visualization tools

Acknowledgments

EGEE III

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COST ESF

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