Earth System Models: Challenges in a changing HPC environment

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Outline

- Introduction

- “Coupling”: An attempt to classify different methods

- Examples, challenges (and solutions)
  1. Atmospheric Chemistry in the Earth System
  2. Atmosphere – Ocean System
  3. On-line nesting: an alternative way to higher resolution

- Summary and Outlook
Computational Earth System Science
(numerical weather prediction and climate simulations)
was from the beginning on exploiting HPC up to the limits …
1950 (Charney, Fjørtoft, von Neumann): first numerical weather forecast on ENIAC (Electronic Numerical Integrator and Computer)

forecast time: 24 hours
computation: 24 hours
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forecast time: 24 hours
computation: 24 hours

2008 (Lynch & Lynch): reconstruction on mobile-phone (JAVA-application):

forecast time: 24 hours
computation: < 1 second (!!!)

http://mathsci.ucd.ie/~plynch/eniac/phonic.html
Deutsches Klimarechenzentrum (DKRZ)

8448 Cores
158 TFlops/s

Top 500
June 2009: no. 27
Nov 2011: no. 98

http://www.dkrz.de
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… mainly for two reasons:

increasing resolution of numerical discretisation(s)
(i.e., finer “grids”)  

increasing complexity by incorporating more and more processes
Computational Earth System Science (numerical weather prediction and climate simulations) was from the beginning on exploiting HPC up to the limits …

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“coupling”
The development of climate models, past, present and future

- Mid-1970s
  - Atmosphere
  - Land surface
  - Ocean & sea-ice

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  - Atmosphere
  - Land surface
  - Ocean & sea-ice

- Early 1990s
  - Atmosphere
  - Land surface
  - Ocean & sea-ice
  - Sulphate aerosol

- Late 1990s
  - Atmosphere
  - Land surface
  - Ocean & sea-ice
  - Sulphate aerosol
  - Non-sulphate aerosol

- Present day
  - Atmosphere
  - Land surface
  - Ocean & sea-ice
  - Sulphate aerosol
  - Non-sulphate aerosol
  - Carbon cycle

- Early 2000s?
  - Atmospheric chemistry
  - Dynamic vegetation

- Ocean & sea-ice model
- Sulphur cycle model
- Land carbon cycle model
- Ocean carbon cycle model
- Atmospheric chemistry

IPCC
INTERGOVERNMENTAL PANEL ON CLIMATE CHANGE
Coupling: circulation of energy, momentum, constituents

Change of state variables by physical, chemical, biological, socio-economic processes
Coupling ...

... the prerequisite is the *operator splitting* concept

(Jöckel et al., ACP, 2005)
Coupling ...  

... the prerequisite is the *operator splitting* concept

Example:

X = air temperature

\[
\frac{\delta X}{\delta t} \quad \text{radiation} \quad \text{convection} \quad \ldots \quad \text{diffusion} \quad \text{time integration}
\]

\(X(t-1)\)

(Jöckel et al., ACP, 2005)
Coupling ... … the prerequisite is the *operator splitting* concept
different numerical algorithms (discretisation, parallel decomposition, cache/vector blocking, ...)

(Jöckel et al., ACP, 2005)
Coupling ...

Example:

basic (dynamical) equations → coupled PDE system

reaction kinetics (chemistry) → coupled ODE system

spectral transform

Rosenbrock-3 (auto)

\[ \frac{\partial X}{\partial t} \]

\[ X(t-1) \]

\[ 0 \]

\[ \text{time integration} \]
Coupling … a classification (of the “way” how operators “communicate”)

- Internal coupling:
  - Os are part of the same program unit (“task”)
  - Data exchange via working memory

- External coupling:
  - Os are split into different program units (“tasks”)
  - Data exchange via external storage (files)

  \[\text{on-line} \quad \rightarrow \quad \text{on-line}\]

  \[\text{off-line} \quad \rightarrow \quad \text{indirect}\]

  \[\text{on-line} \quad \rightarrow \quad \text{direct}\]

  \[\text{off-line} \quad \rightarrow \quad \text{indirect}\]

- Involves an add. external program (“coupler”)
Coupling ... a classification

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- Data exchange via working memory
  - Off-line: indirect
  - On-line: direct

Choice depends on:
- Application
- Implementation effort (legacy code!)
- Desired sustainability, flexibility, re-usability
- Compromise in minimizing computational and communication overheads

→ Involves an add. external program ("coupler")
Example 1: internal coupling

Language level:

CALL subroutine_1( ..., A, ...) [INTENT(OUT)]

CALL subroutine_2( ..., A, ...) [INTENT(IN)]

more formal: standard model infrastructure + coding standard

- Earth System Modeling Framework (ESMF)  
  (http://www.earthsystemmodelling.org)
- Modular Earth Submodel System (MESSy)
  (http://www.messy-interface.org, Jöckel et al., ACP, 2005)
- ... (many others)

key: strict separation of model infrastructure (4 layer!)
  (memory management, I/O, parallel decomp., time control, etc.)
  from “process” (and “diagnostic”) formulations
Example 1a: **internal coupling** of Atmospheric Chemistry in MESSy

coupling via model infrastructure (nearly object oriented)
- TIMER
- CHANNEL (pointer based memory management and I/O)
- TRACER (special for chemical constituents)
- ...

“operators” = “processes” = “submodels”
photo-chemistry:
...
A + B → C + D :: J(light, ...)
B + E → F + G :: k(p, T, ...)
...

==> ODE system
Number* of sub-time steps of the ODE solver for the kinetic system

T106L90MA → ~ 1.125° x 1.125° x 90 (~80 km) ; Δt = 6 min
Number of sub-time steps of the ODE solver for the kinetic system

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*vertical average
Number* of sub-time steps of the ODE solver for the kinetic system

T106L90MA $\rightarrow$ $\sim 1.125^\circ \times 1.125^\circ \times 90$ ($\sim 80$ km); $\Delta t = 6$ min

*vertical average

Load imbalance due to time dependent stiffness of kinetic (ODE) system $\rightarrow$ possible solution: dynamic parallel decomposition
Example 2: **internal coupling** versus **indirect external coupling** of an Atmosphere – Ocean System (domain coupling)

MPIOM as MESSy submodel
“coupled to” ECHAM5

MPIOM – OASIS3 – ECHAM5
Example 2: internal coupling versus indirect external coupling of an Atmosphere – Ocean System (domain coupling)
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grid-trafo (semi-parallel)

“all-gather”

“gather”

incl. grid-trafo (serial)

“scatter”
Example 2: Performance (seconds per simulated month)

\[ Y = 0.89207 \times X \]
\[ R^2 = 0.9984 \]

depends on:
- HPC system
- model setup

(Pozzer et al., GMD, 2011)
Example 3: On-line nesting: an alternative way to higher resolution

- 1-way on-line nested global-regional atmospheric model system (zoom)

- multiple instances possible due to client – server architecture of MMD ...

MECO(n):
MESSy-fied ECHAM and COSMO models n-times nested

(Kerkweg & Jöckel, GMD, 2012a,b; Hofmann et al., GMD, 2012)
MECO(2) simulation of Eyjafjallajökull eruption plume 2010

TIME: 17-APR-2010 00:00  column density [arbitrary units]

EMAC T106L31 ECMWF
(1.125° x 1.125°, 6 min)

COSMO/MESSy-EU
(40 km, L40, 3 min)

COSMO/MESSy-DE
(7 km, L40, 40 sec)

(c) Patrick Joeckel, DLR, Aug 2011
Example 3: On-line nesting: an alternative way to higher resolution

MMD-Server (ECHAM5 or COSMO)  MMD-Client (COSMO)

server tasks

memory buffers

client tasks

MPI based, single sided “point-to-point” communication between c&s tasks with overlapping grids
Example 3: On-line nesting: an alternative way to higher resolution

(Kerkweg & Jöckel, GMD, 2012b)
Example 3: On-line nesting: an alternative way to higher resolution

<table>
<thead>
<tr>
<th>No. of Tasks</th>
<th>ECHAM-COSMO-40 km</th>
<th>COSMO-7 km</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-4-24</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4-4-56</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4-4-88</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4-4-120</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

4-4-56 is most efficient!

Additional effort to optimize efficiency!
Summary

- ESMs are computationally demanding due to *continuously increasing complexity*
- *Operator splitting* is basis for coupling of model components
- Different coupling methods exist;
  challenge: efficiency – computation versus communication
- Exemplary challenges:
  - Atmospheric Chemistry: *internal coupling*
    → Load Imbalance (parallel decomp.)
  - Atmosphere – Ocean System: *internal* vs. *indirect external* coupling
    → both feasible, best choice depends on model (legacy code!), model setup, HPC-system
  - Global – Regional Nesting: *direct on-line coupling* (client – server approach)
    → complex timing, add. effort to achieve efficiency
- (exascale parallelisation, parallel I/O, memory/core reduction)