Making extreme computations possible with virtual machines

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Chokoufé/Ohl/JRR, Comput.Phys.Commun. 196 (2015) 58-69

HELMHOLTZ
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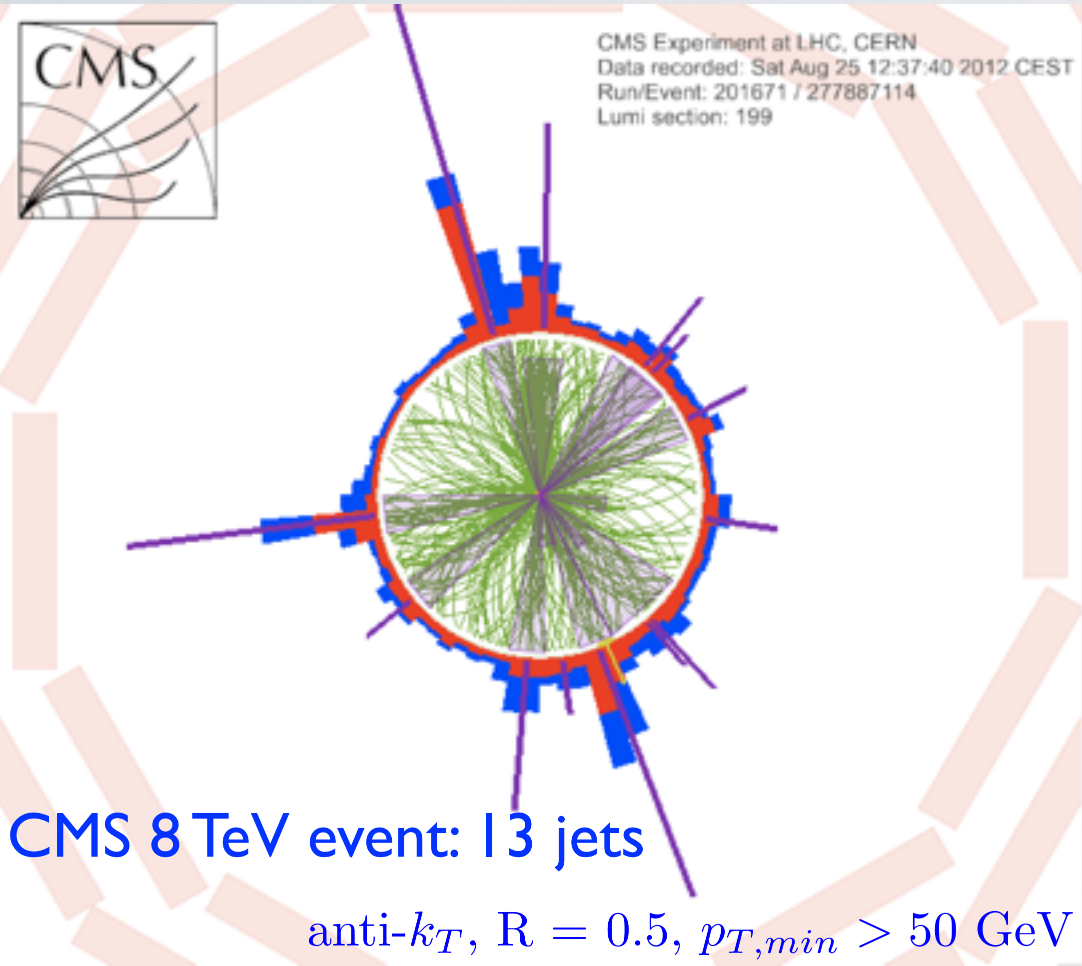
Motivation: why extreme computations?



CMS 8 TeV event: 13 jets

anti-k_T, R $= 0.5$, $p_{T,min} > 50$ GeV

- Modern collider experiments need matrix elements (MEs) of tremendous multiplicity
- Tree-level MEs needed in corrections to the parton shower (merging) and for *k* real emissions in N^{k}LO fixed order calculations
- Examples: access to top Yukawa at ILC/CLIC:

$$\begin{aligned} e^+e^- &\to \quad bbbb + 4j \\ e^+e^- &\to \quad bb\ell\nu_\ell + 6j \\ e^+e^- &\to \quad bb + 8j \end{aligned}$$

- Automated efficient ME generators provide every multiplicity (*in principle*) `Alpha` [Caravaglios/Moretti, 1995], `O'Mega` [Ohl/JRR, 2000], `Helac` [Papadopoulos, 2001], `Comix` [Gleisberg/Hoeche, 2008]

- Direct numerical implementations of recursions less flexible
- Traditional method: use meta programming to combine fast code & full flexibility
  - Algebraic expression from high-level language: `Form`, `Mathematica`, `OCaml`, `Python`, ...
  - Evaluation in numerical fast language: `C`, `Fortran`, ...
  - Examples: `O'Mega` [Ohl/JRR, 2000], `Madgraph` [Alwall et al., 2008], `FormCalc` [Hahn/Perez-Victoria, 1998], `GoSam` [van Deurzen et al., 2013], ...

What to do with complex processes?

- BUT: analytic expressions of complex (multi-jet) processes can reach GiB size,
- $gg \to 6g$ reaches size of 4 GB in `O'Mega` [Kilian/Ohl/JRR/Speckner, 1206.3700]
- No hope for higher multiplicities …
- Possible solution: Virtual Machine (VM) circumvents compilation of large code completely
- VM easy to implement and parallelize, similar performance than compiled code
- VM is no OS emulation in this context … … … [Chokoufé/Ohl/JRR, 1411.3834]

What is a Virtual Machine (VM)

☐ A Virtual Machine (VM) in our context is a compiled program (interpreter)

☐ The VM is able to read instructions from disk

☐ The VM performs arbitrary number of operations of a finite instruction set

☐ Instructions can be stored as byte code (encoded as numbers in ASCII file)

☐ VM can be regarded as machine with registers and instructions what to do on the registers

☐ Similar to a CPU, but on a higher level:

registers are e.g. arrays of momenta and wave functions

instructions are e.g. scalar products of momenta and wave functions

Contents of the byte code

- VM should be constructed dynamically (for user-defined processes)
- $\Longrightarrow$ provide header with number of objects to be allocated
- [optionally: version numbers to specify the physical model, comments on the creation of the byte code, tables with precomputed properties (information over helicity, color, flavor]
- Then: body of instructions (non-trivial information how to compute a process)
- First object of instruction is the opcode: specifies which operation is executed

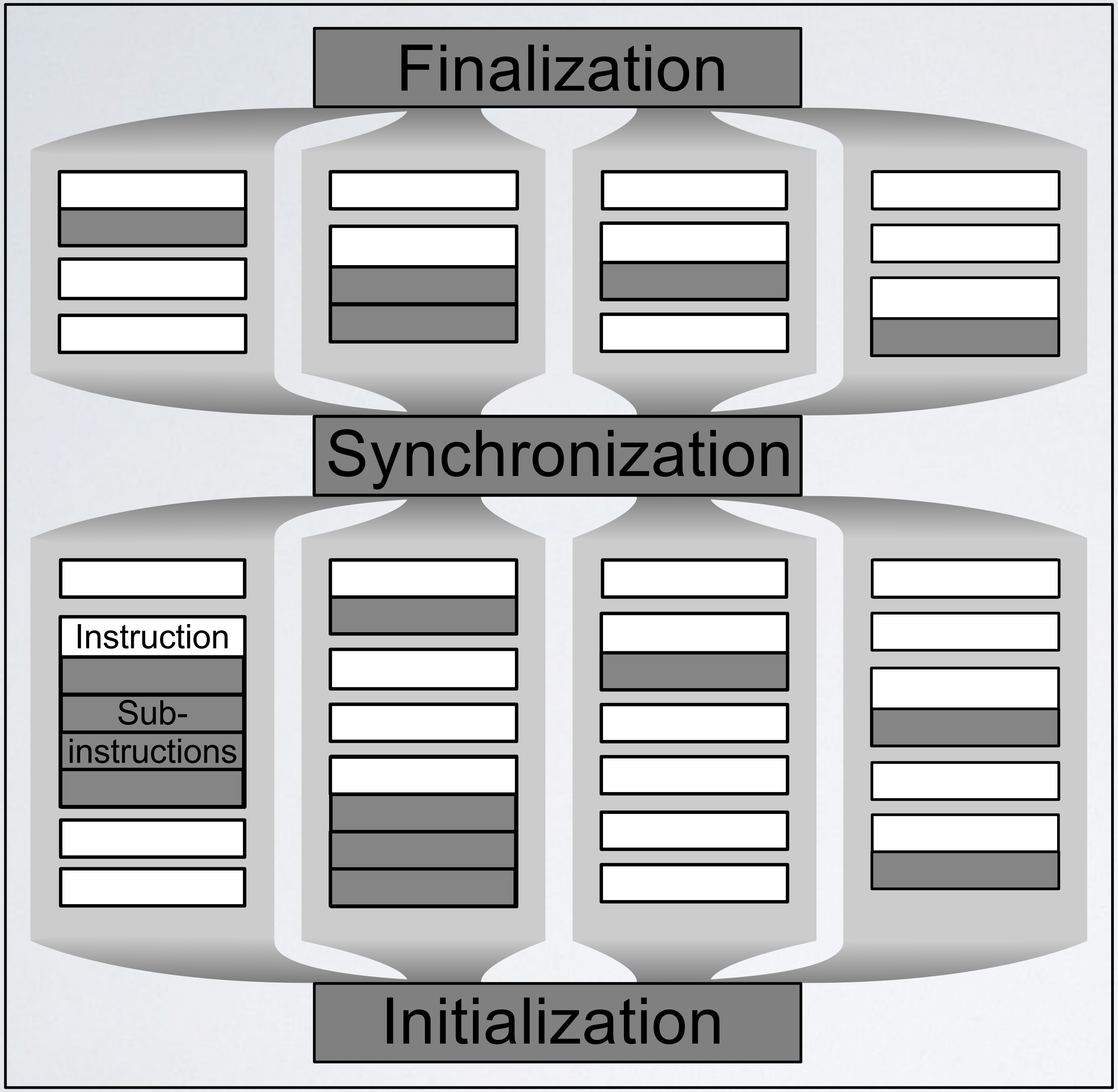
usually by addresses of registers, for example:

```
1 7 4 3    ⇔    momentum(7) = momentum(4) + momentum(3)
```

Interpreter (VM *per se*)

- Simple (compiled) program: reads first byte code into memory
- VM decode function loops over instructions with given input values
- Translation of byte code to machine code (very) fast compared to execution
  (execution consists of large number of complex scalar products)
- Adapting interpreter to a new process/matrix element requires
  - Specification of static information (spin tables, color tables etc.)
  - Writing the selection statements for the decode function
- VM is compiled once fast: handy for validation (checking many small processes), inevitable for (very) large processes

Parallelization in the Virtual Machine



- Group instructions into building blocks: minimize number of synchronization points

- Divide computation into levels

- All building blocks commute in every level

  (i.e. only one thread is writing to register per level)

Parallelization in High Energy Physics

- Usual assumption: trivial parallelizability of computations by computing multiple phase space points at once
  (phase space integration ≡ momenta, helicities, colors, flavors)

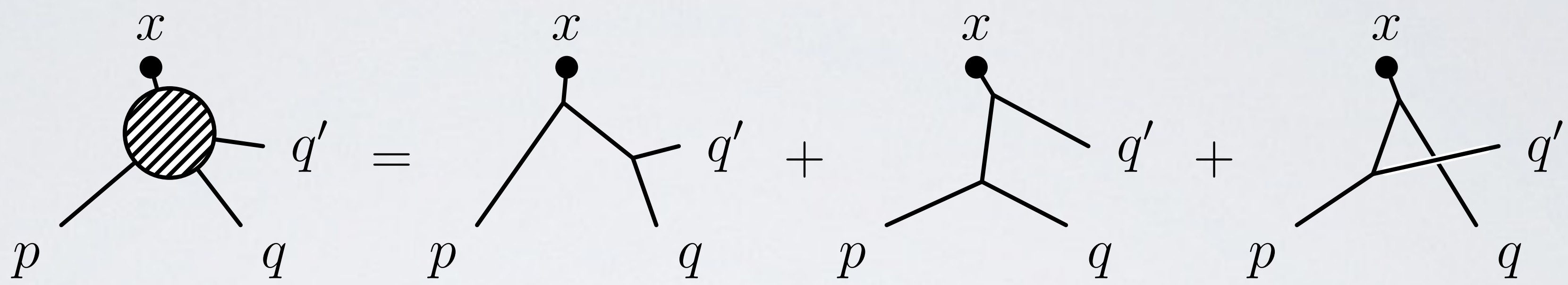
- Extreme computations: objects of single phase space point might already fill up your cache)

- Computing multiple points at once can induce traffic jam between RAM and CPU ⟹ might even be slower than single core performance

- VM is a straightforward implementation of the
  parallel computation of a single phase space point

The Optimizing Matrix Element Generator (`O'Mega`)

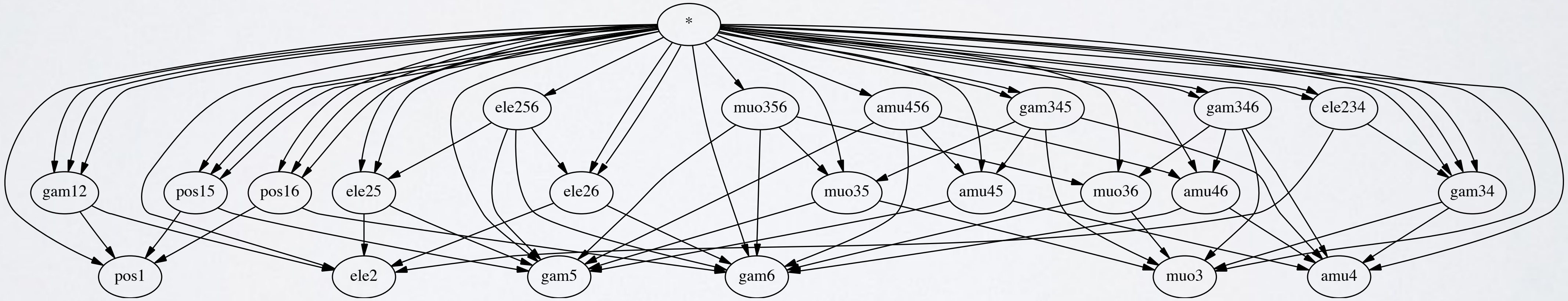
- `O'Mega` [Ohl, 2000; Moretti/Ohl/JRR, 2001; JRR, 2002] computes amplitudes with 1-particle off-shell wave functions (1POWs)



- Possible to construct set of all currents recursively (tree-/1-loop level)

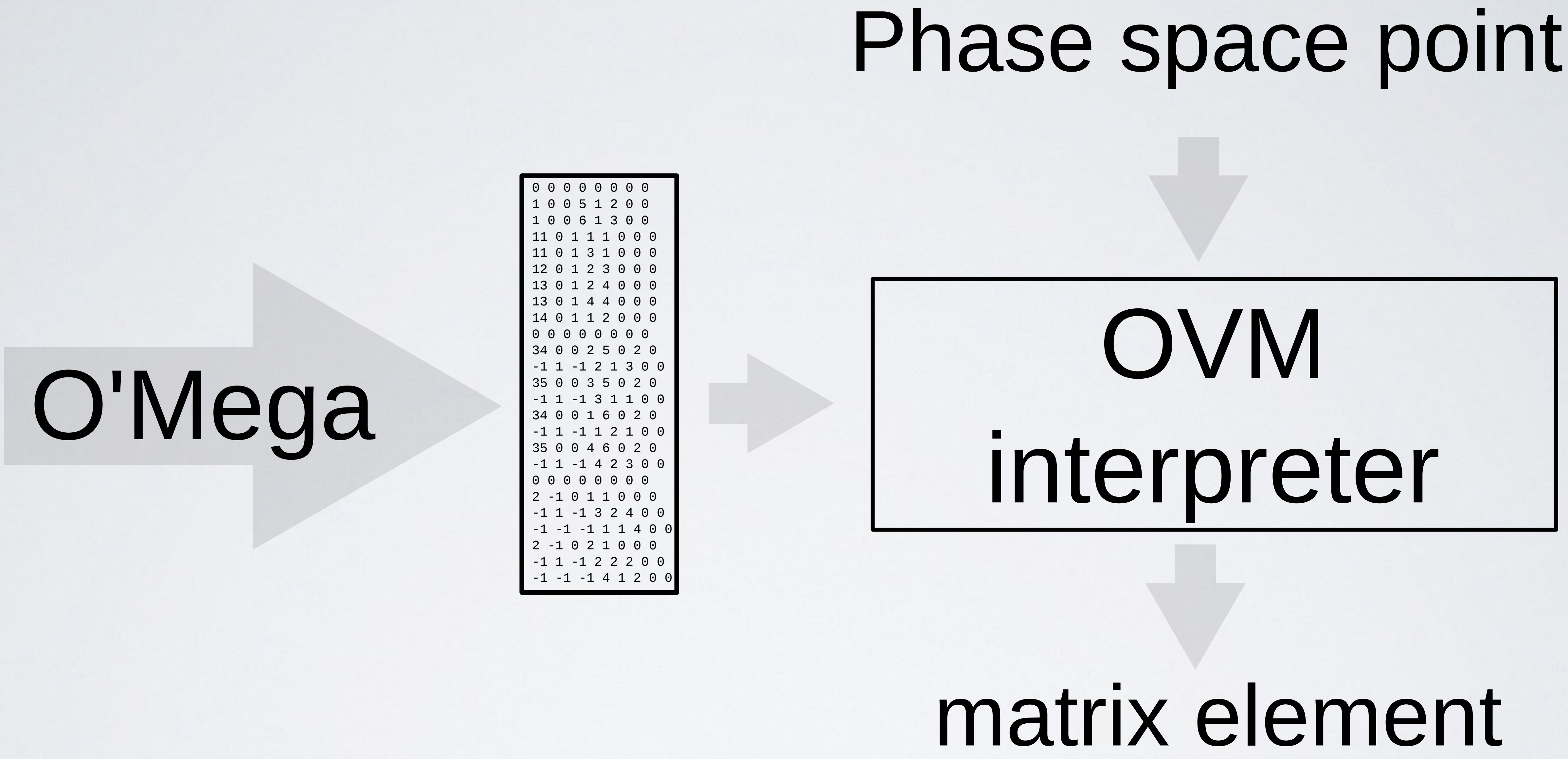
- Keystones *K* to replace sum over Feynman diagrams

$$\sum_{i=1}^{F(n)} D_i = \sum_{k,l,m=1}^{P(n)} K^{(3)}_{f_k f_l f_m}(p_k, p_l, p_m) W_{f_k}(p_k) W_{f_l}(p_l) W_{f_m}(p_m)$$



- Calculation forms Directed Acyclical Graphs (DAGs), optimized to consist only of the minimal number of connections by `O'Mega`

Layout of the general infrastructure



O'Mega

```
0 0 0 0 0 0 0 0
1 0 0 5 1 2 0 0
1 0 0 6 1 3 0 0
11 0 1 1 1 0 0 0
11 0 1 3 1 0 0 0
12 0 1 2 3 0 0 0
13 0 1 2 4 0 0 0
13 0 1 4 4 0 0 0
14 0 1 1 2 0 0 0
0 0 0 0 0 0 0 0
34 0 0 2 5 0 2 0
-1 1 -1 2 1 3 0 0
35 0 0 3 5 0 2 0
-1 1 -1 3 1 1 0 0
34 0 0 1 6 0 2 0
-1 1 -1 1 2 1 0 0
35 0 0 4 6 0 2 0
-1 1 -1 4 2 3 0 0
0 0 0 0 0 0 0 0
2 -1 0 1 1 0 0 0
-1 1 -1 3 2 4 0 0
-1 -1 -1 1 1 4 0 0
2 -1 0 2 1 0 0 0
-1 1 -1 2 2 2 0 0
-1 -1 -1 4 1 2 0 0
```

Phase space point

OVM
interpreter

matrix element

Byte code generation in `O'Mega/OCaml`

- Feynman rules form finite set of instructions
- Good candidates for translation into byte code
- Ordering of instructions needed
- `OCaml` compares abstract objects (wave functions, momenta, amplitudes)
- `Fortran` arrays ordered according to their index position
- Take set of objects: apply mapping to natural numbers using the given order

code	coupl	coeff	lhs	rhs$_1$	rhs$_2$	rhs$_3$	rhs$_4$
ADD_MOMENTA	0	0	p_lhs	p_rhs$_1$	p_rhs$_2$	p_rhs$_3$	0
LOAD_X	PDG	0	wf	outer_ind	0	0	amp
PROPAGATE_Y	PDG	width	wf	p	0	0	amp
FUSE_Z	coupl	coeff	lhs	rhs$_1$	rhs$_2$	rhs$_3$	rhs$_4$
CALC_BRAKET	sign	0	amp	sym	0	0	0

Performance of byte code generation

- ☑ Byte code is produced faster than compiled code
- ☑ Byte code uses less RAM than compiled code
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process	`BC` size	`Fortran` size	t_{compile}
$gg \to gggggg$	428 MB	4.0 GB	-
$gg \to ggggg$	9.4 MB	85 MB	483(18) s
$gg \to q\bar{q}q'\bar{q}'q''\bar{q}''g$	3.2 MB	27 MB	166(15) s
$e^+e^- \to e^+e^-e^+e^-e^+e^-e^+e^-e^+e^-$	0.7 MB	1.9 MB	32.46(13) s

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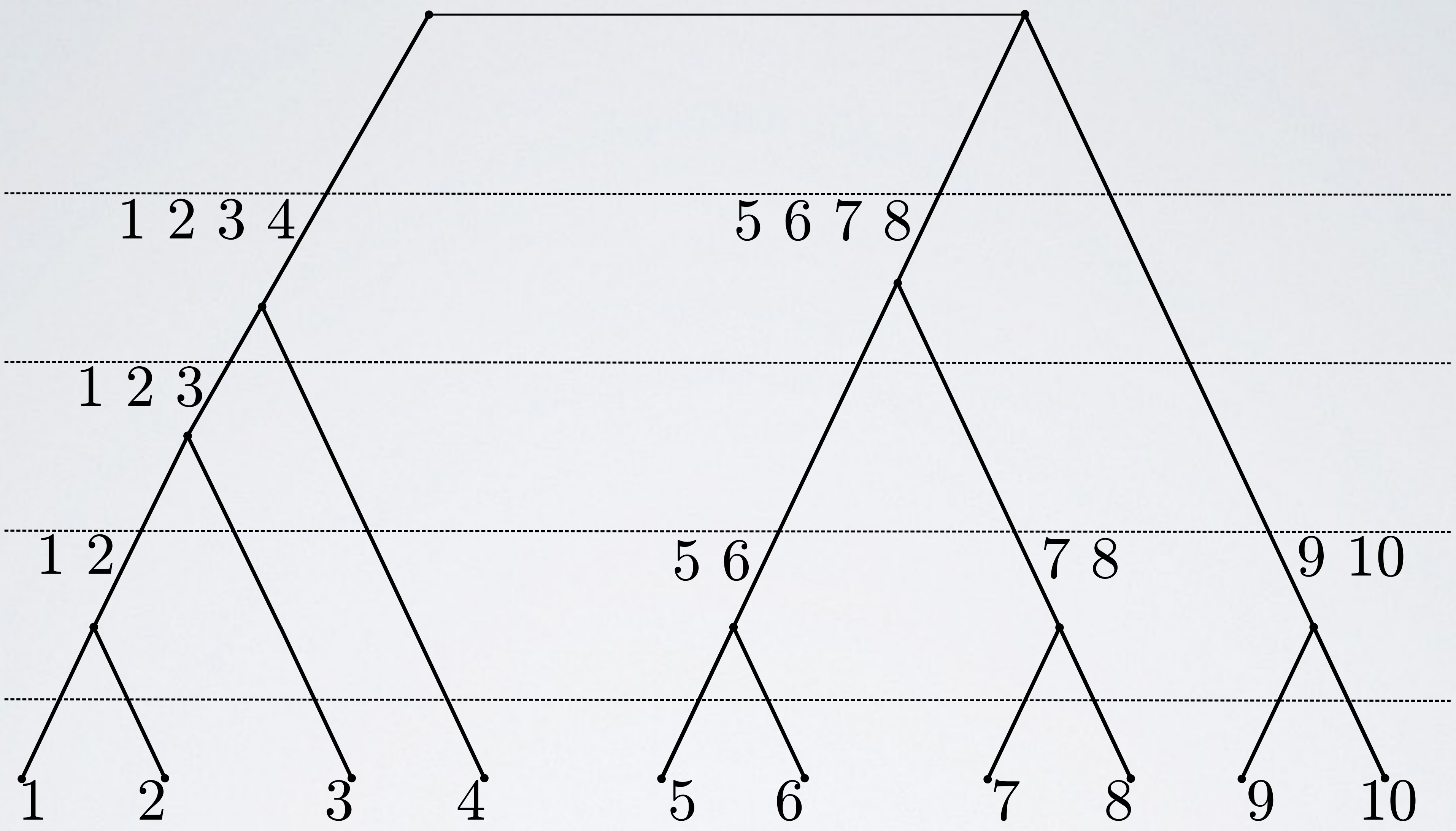
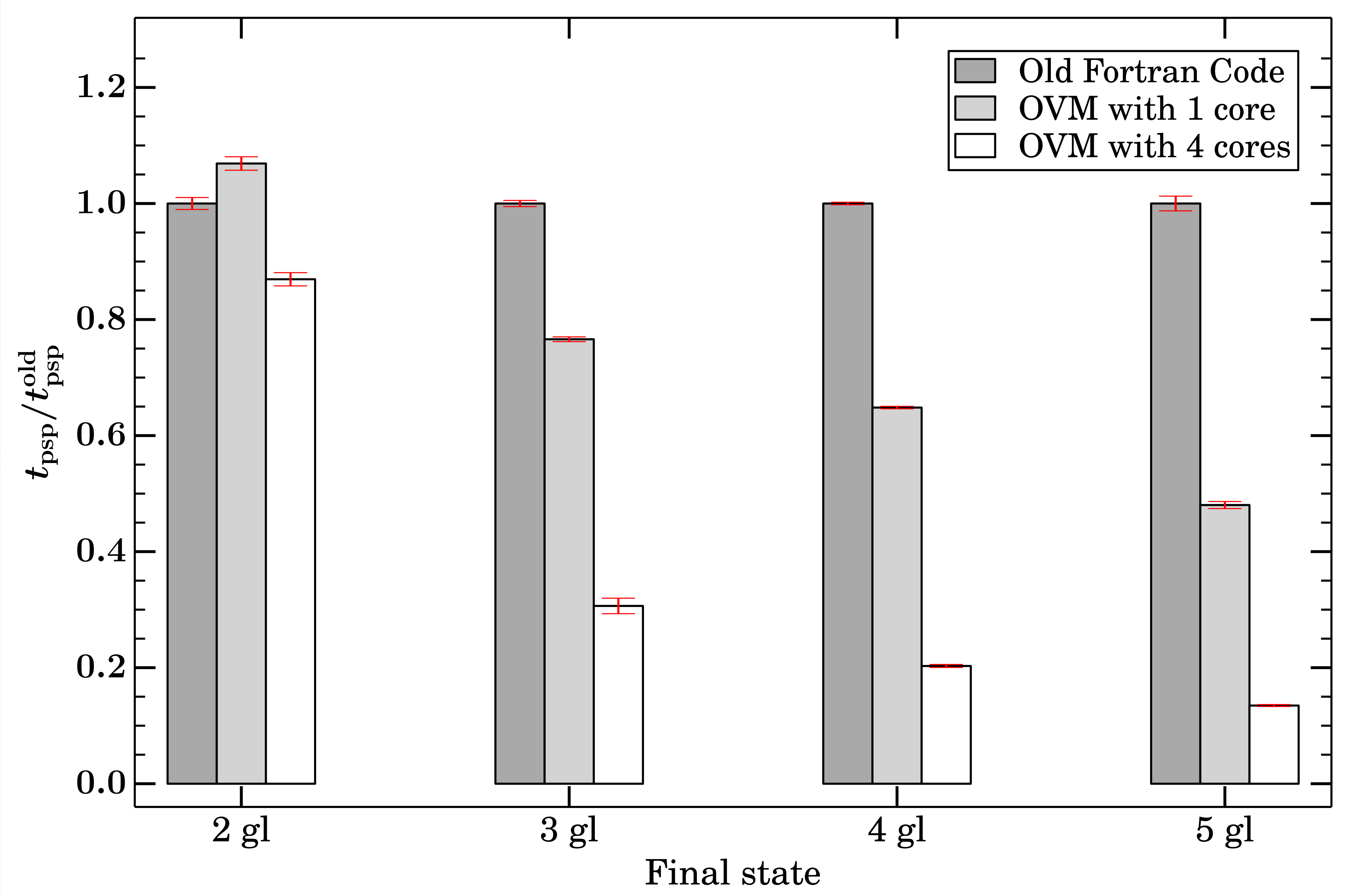
- ☑ No big changes for smaller processes

Parallelization in recursive computations



Identify a level of the parallelization by counting external momenta

Speed of VM matrix elements — First glance

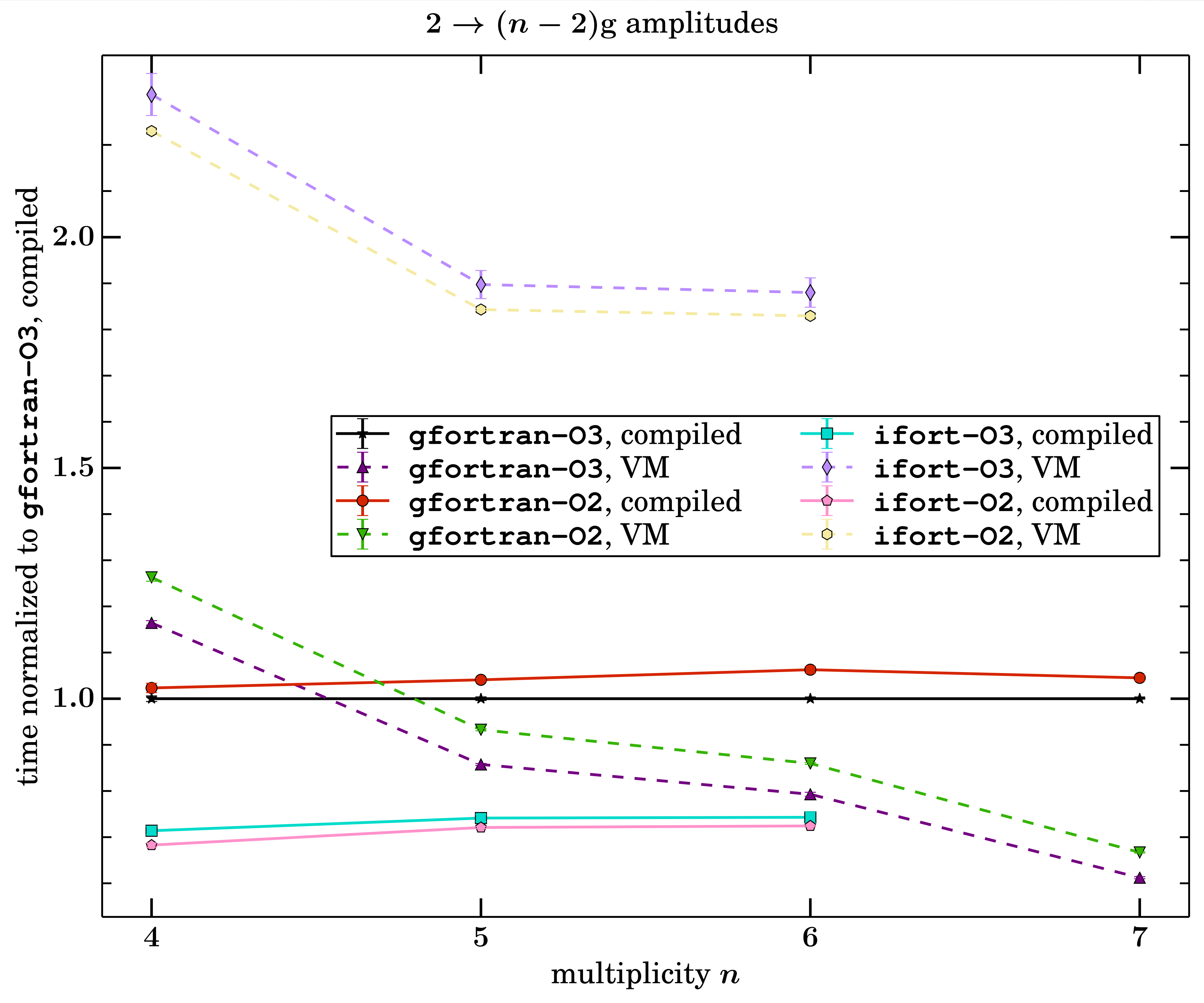


`[gfortran 4.7.4, Intel i7-2720QM @ 2.2 GHz]`

Speed of matrix elements — w/ two compilers

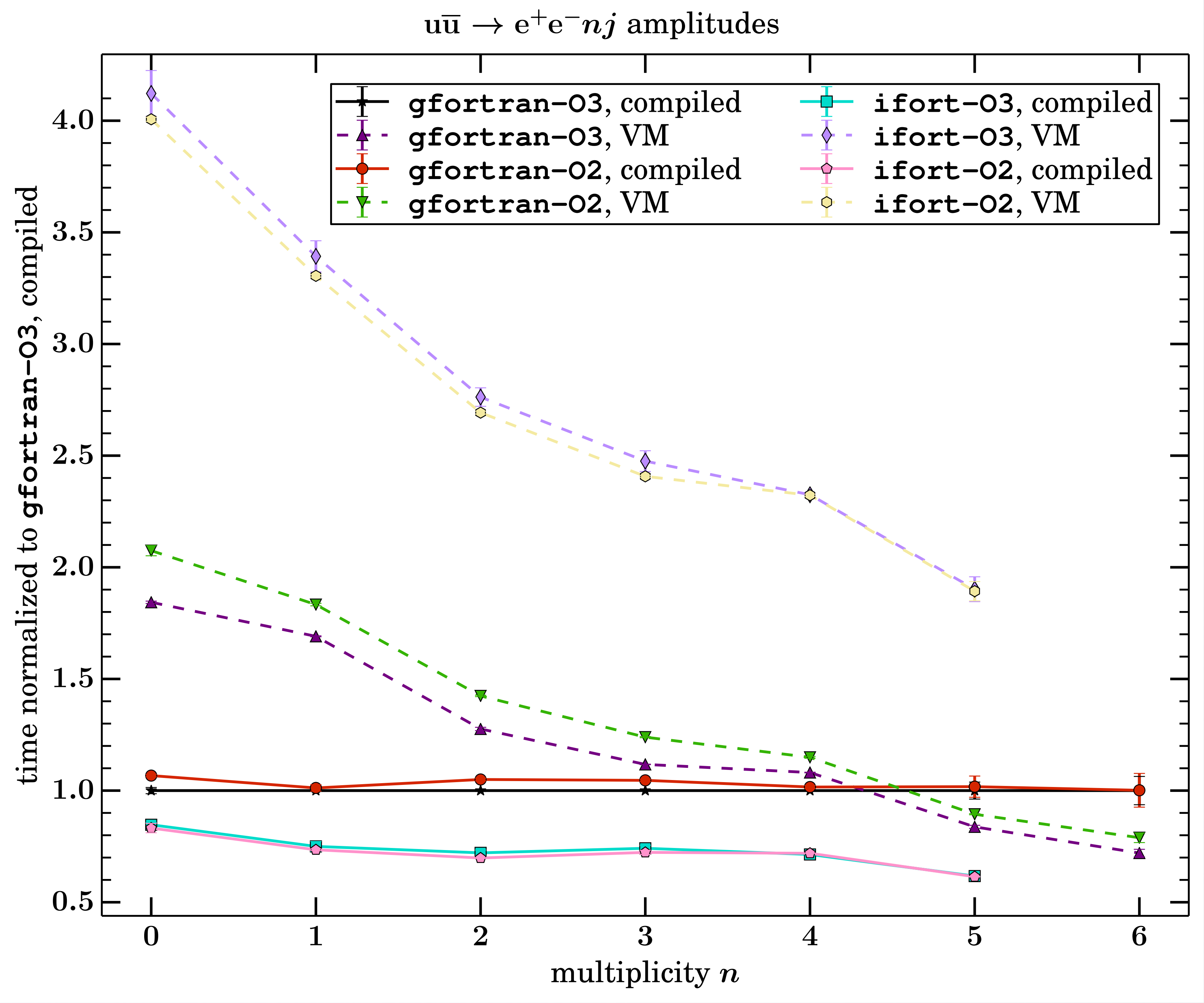
[`gfortran 4.7.4`/`ifort 14.0` on
`Intel Xeon E5-2440 @ 2.4 GHz`]

- Both VMs improve with increasing multiplicity
- ifort has large offset for the VM: needs profile-guided optimization to resolve
- `ifort v14.0` fails to compile 2 → 5 gluon amplitude
  (even with `-O0`)



Speed of matrix elements — explaining the Scaling

- Same scaling behavior
- Virtualisation costs constant
- VM does loop over levels and instructions in the levels
- Source code is like an unrolled version of this loop
- Double loop of VM has higher probability to keep decode function in instruction cache

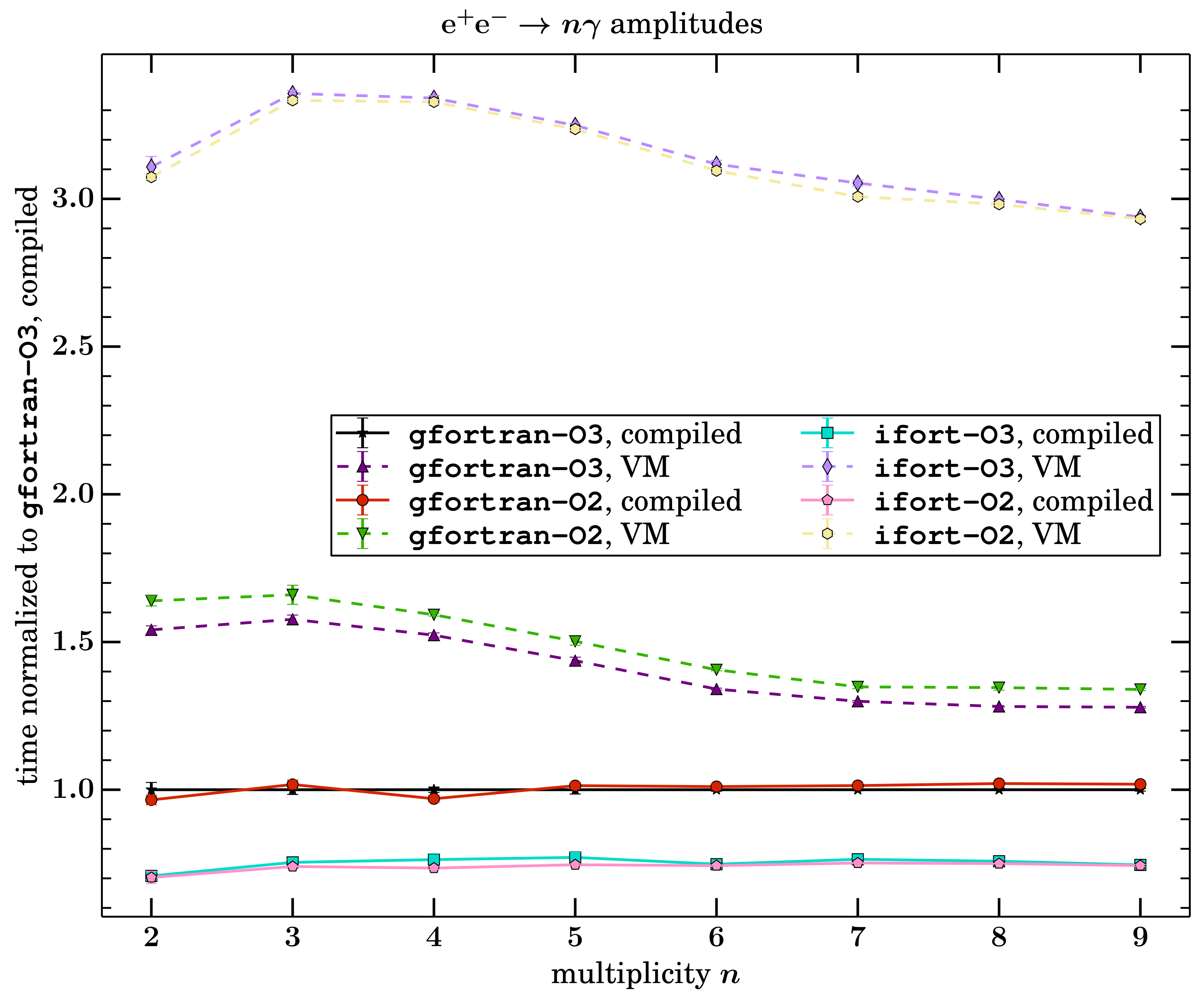


Speed of matrix elements

- For pure QED with increasing multiplicity: Improvements in VM smaller
- More wave functions per level: less to be done!
- Unrolled version can gain more from prefetching
- Be aware of the size:

  $e^+e^- \to 9\gamma$ 125 KiB

  $gg \to 4g$ 269 KiB



Quantitative Analysis of the Parallelization

- **Amdahl's Law** divides an algorithm into a parallelizable part *p* and strictly serial parts 1 - *p*

- **Amdahl's Law** determines possible speedup *s* for a computation with *n* cores

  Consider the time on 1 and *n* cores, resp.: $t^{(1)}, t^{(n)}$

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- Compare parallelization of the amplitude (A) with parallel computation of single complete phase space points (P)

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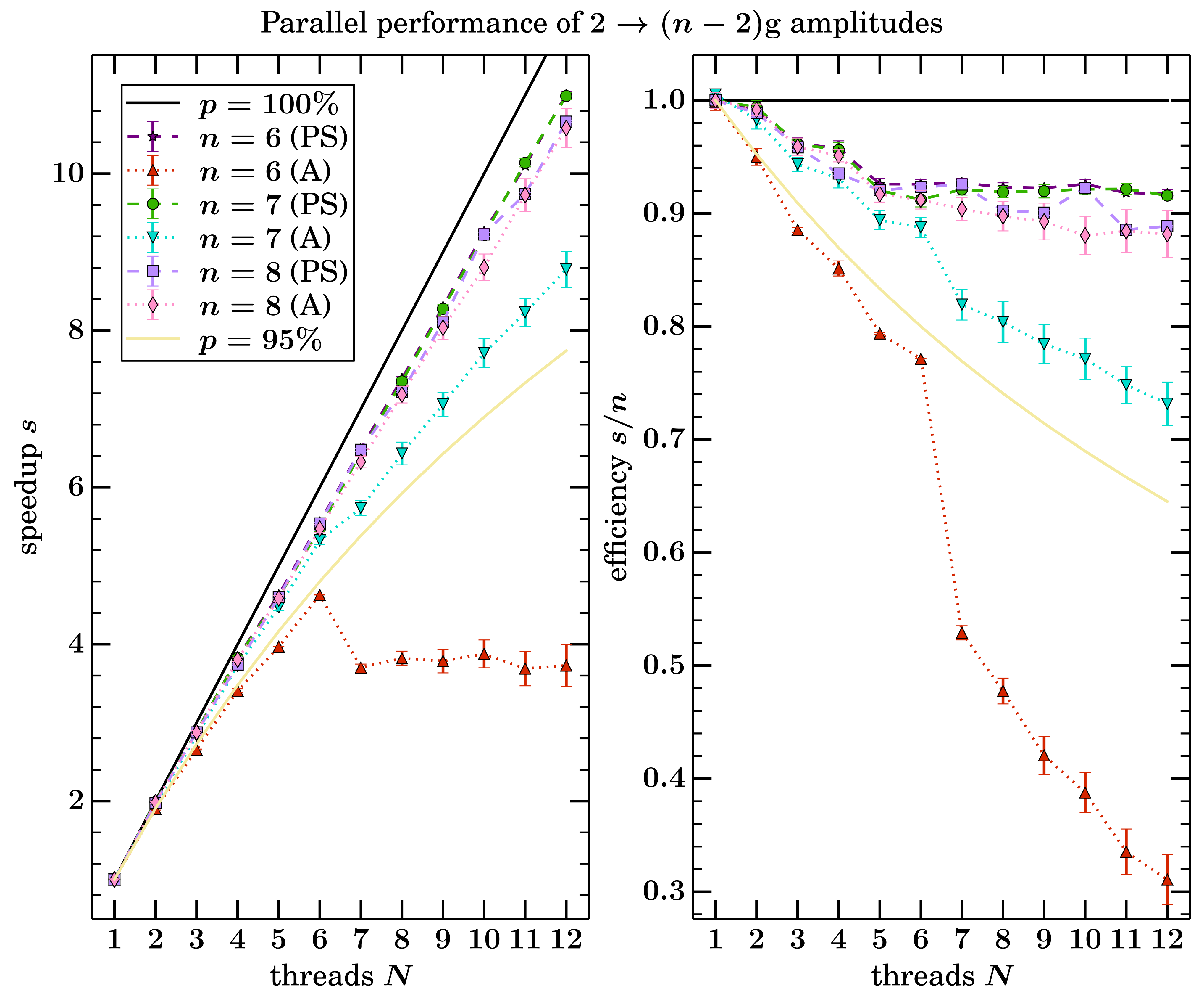

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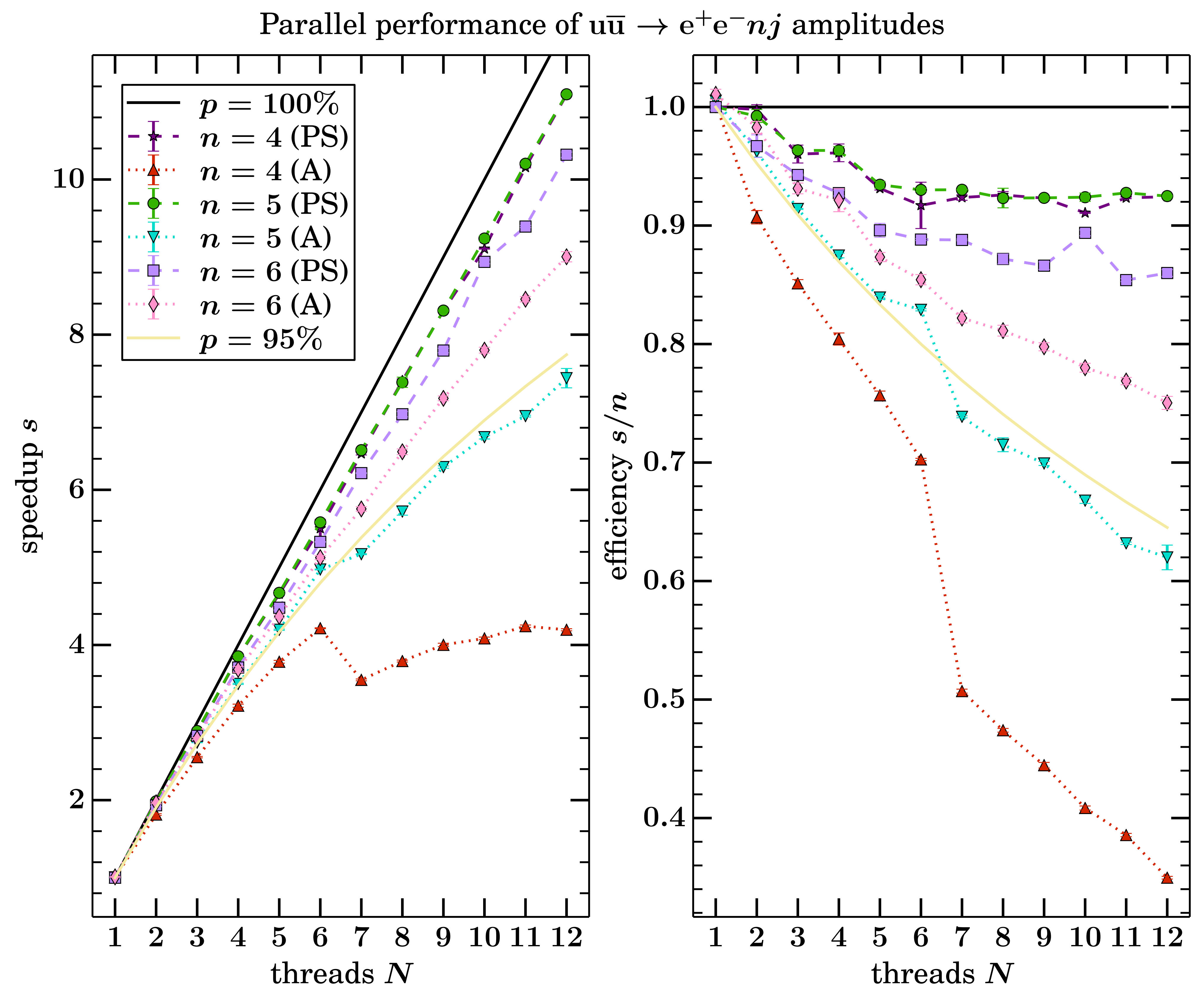

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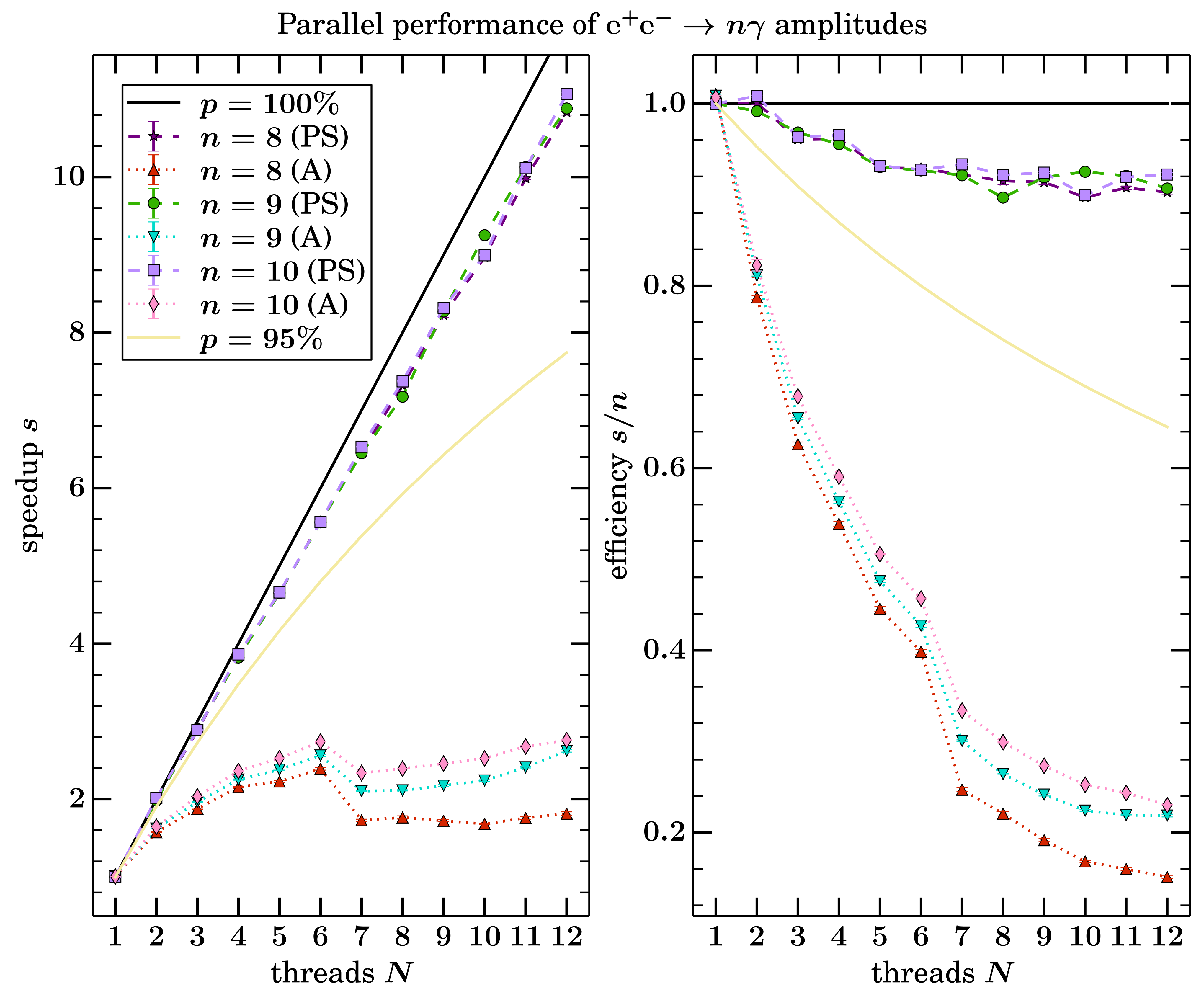


Implementation / Usage in WHIZARD

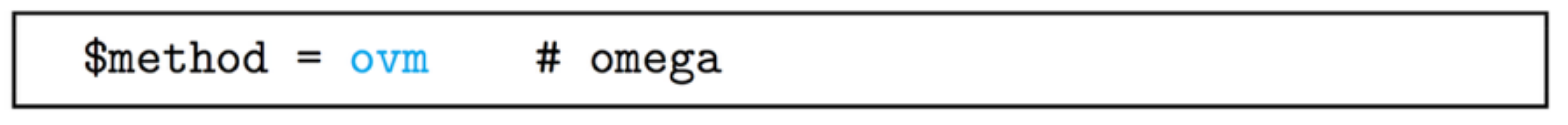
WHIZARD v2.2.8 (22.11.2015) *http://whizard.hepforge.org* <*whizard@desy.de*>

WHIZARD Team: *Wolfgang Kilian, Thorsten Ohl, JRR, Simon Braß/Bijan Chokoufé/Marco Sekulla/Soyoung Shim/Florian Staub/Christian Weiss/Zhijie Zhao* + *2 Master*

EPJ C71 (2011) 1742

- Universal event generator for lepton and hadron colliders
- Modular package:
  - Phase space parameterization (resonances, collinear emission, Coulomb etc.)
  - O'Mega optimized matrix element generator (recursiveness via Directed Acyclical Graphs)

    Compiled matrix element code & O'Mega Virtual Machine (OVM)
  - Color flow formalism Stelzer/Willenbrock, 2003; Kilian/Ohl/JRR/Speckner, 2011
  - VAMP: adaptive multi-channel Monte Carlo integrator
  - CIRCE1/2: generator/simulation tool for lepton collider beam spectra
  - Lepton beam ISR Kuraev/Fadin, 2003; Skrzypek/Jadach, 1991



```
$method = ovm     # omega
```

Available for the following models:

`SM, SM_CKM, SM_Higgs, Zprime, QCD, QED, 2HDM, 2HDM_CKM, HSExt`

Application on GPUs ?

- GPUs allow highly efficient 4-vector calculations (speed-ups of 50-100 reported)
- GPUs suffer from problem of finite (small) size of its kernel
- VM could be the perfect tool for such computations
- Existing studies: performance degrades with growing multiplicity ⟹ code has to be split into smaller programs [Hagiwara/Kanzaki/Li/Okamura/Stelzer, 1305.0708]
- Decode function of VM remains sufficiently small
- Possible remaining obstacle: Efficiency of memory management
- Reduce communication costs: transfer instructions and VM to GPU only once
- Strategy:

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- Possible remaining obstacle: Efficiency of memory management
- Reduce communication costs: transfer instructions and VM to GPU only once
- Strategy:
  - Send only quantum numbers and momenta to GPU
  - Receive the amplitudes as complex numbers from the GPU
  - Phase space integration / reweighting etc. happens on the CPU

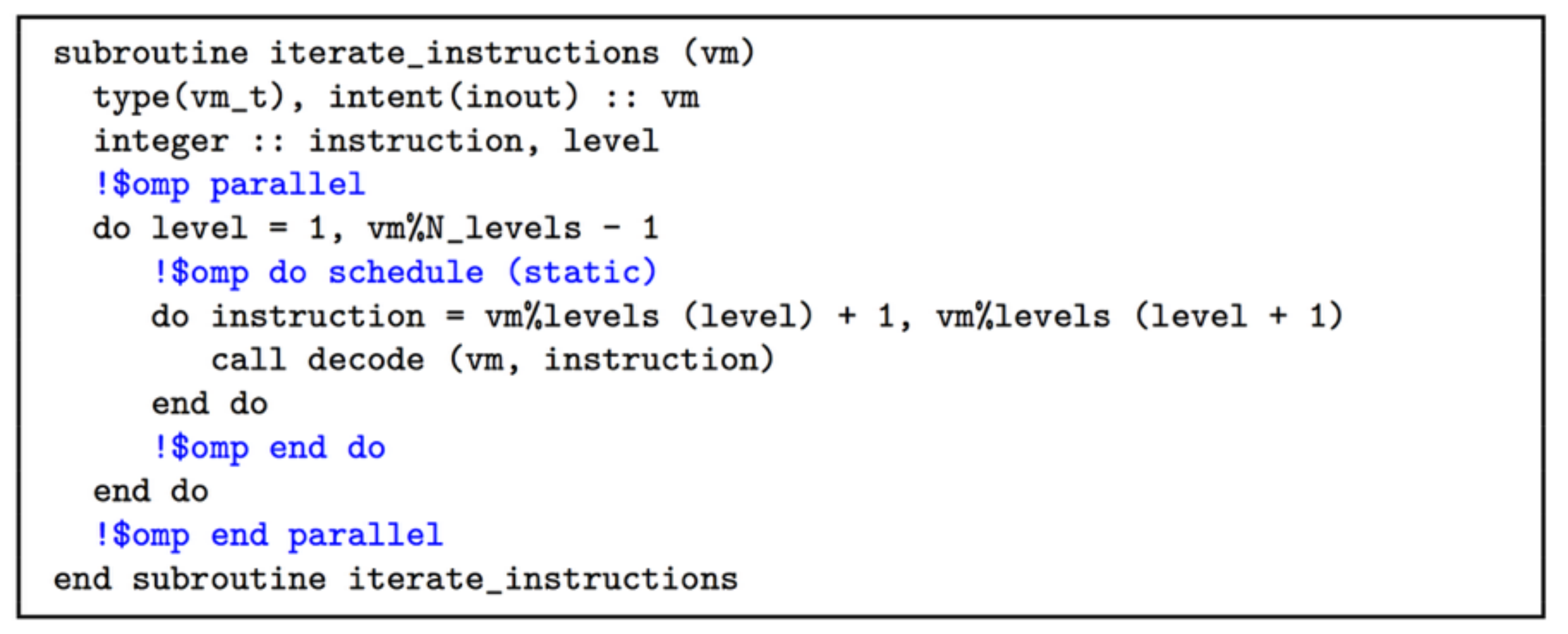
Conclusions & Outlook

- Virtual Machines allow to compute directly
- No compile time needed (hours/days for complicated processes)
- Implementation for High Energy Physics: O'Mega Virtual Machine

  [Chokoufé/Ohl/JRR, Comput.Phys.Commun. 196 (2015) 58-69]
- OVM included in event generator `WHIZARD 2.2`
- (Very) complicated processes benefit from/need parallelization of single phase space points   straightforward in the VM
- Execution times same order as compiled code (sometimes even faster)
- Might allow to run on graphic cards: ME [OVM] on GPU, MC core on CPU
- Idea very general: summation, algebraic operations, etc.

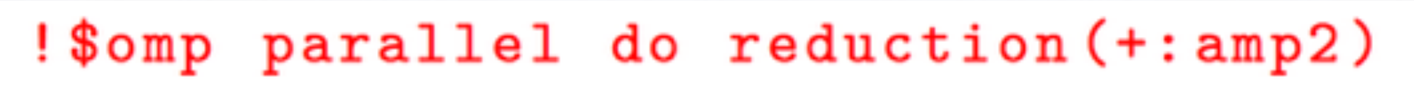
BACKUP SLIDES

Implementation of (OMP) parallelisation



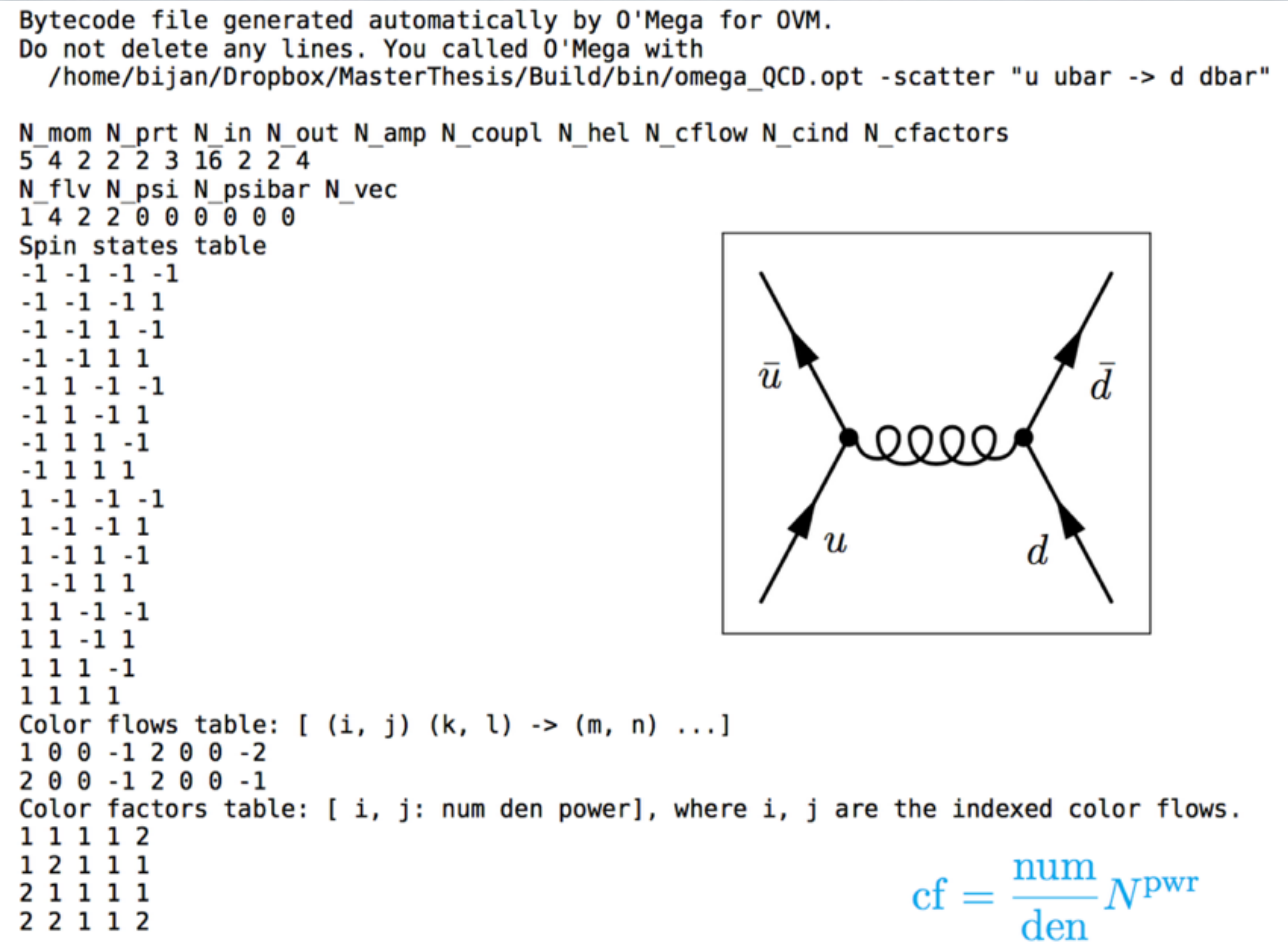
```
subroutine iterate_instructions (vm)
  type(vm_t), intent(inout) :: vm
  integer :: instruction, level
  !$omp parallel
  do level = 1, vm%N_levels - 1
     !$omp do schedule (static)
     do instruction = vm%levels (level) + 1, vm%levels (level + 1)
        call decode (vm, instruction)
     end do
     !$omp end do
  end do
  !$omp end parallel
end subroutine iterate_instructions
```

Also the color sum has to be parallelized, too:



```
!$omp parallel do reduction(+:amp2)
```

Byte code in detail

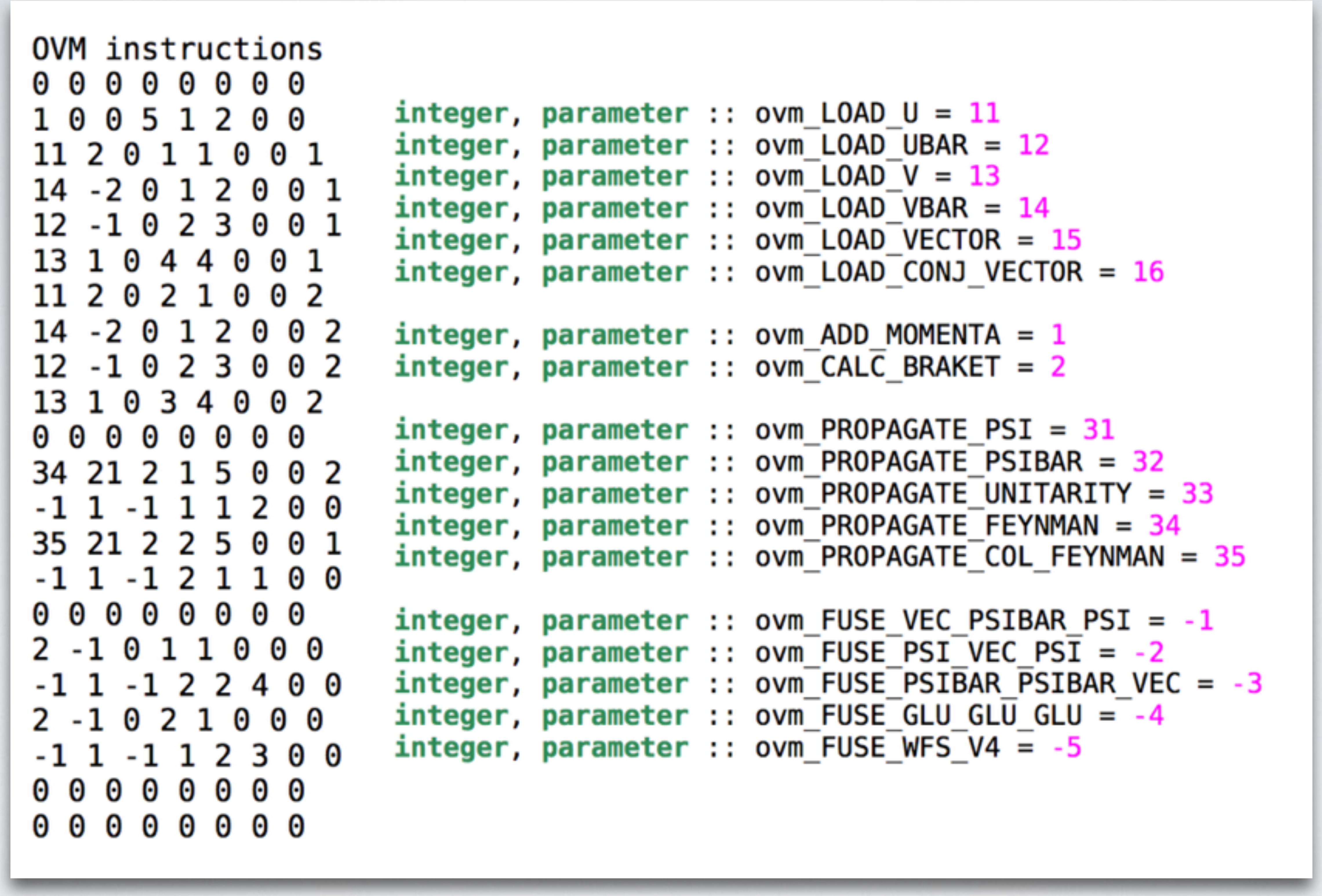


```
Bytecode file generated automatically by O'Mega for OVM.
Do not delete any lines. You called O'Mega with
  /home/bijan/Dropbox/MasterThesis/Build/bin/omega_QCD.opt -scatter "u ubar -> d dbar"

N_mom N_prt N_in N_out N_amp N_coupl N_hel N_cflow N_cind N_cfactors
5 4 2 2 2 3 16 2 2 4
N_flv N_psi N_psibar N_vec
1 4 2 2 0 0 0 0 0 0
Spin states table
-1 -1 -1 -1
-1 -1 -1 1
-1 -1 1 -1
-1 -1 1 1
-1 1 -1 -1
-1 1 -1 1
-1 1 1 -1
-1 1 1 1
1 -1 -1 -1
1 -1 -1 1
1 -1 1 -1
1 -1 1 1
1 1 -1 -1
1 1 -1 1
1 1 1 -1
1 1 1 1
Color flows table: [ (i, j) (k, l) -> (m, n) ...]
1 0 0 -1 2 0 0 -2
2 0 0 -1 2 0 0 -1
Color factors table: [ i, j: num den power], where i, j are the indexed color flows.
1 1 1 1 2
1 2 1 1 1
2 1 1 1 1
2 2 1 1 2
```

$$\mathrm{cf} = \frac{\mathrm{num}}{\mathrm{den}} N^{\mathrm{pwr}}$$

Byte code in detail



```
OVM instructions
0 0 0 0 0 0 0 0
1 0 0 5 1 2 0 0
11 2 0 1 1 0 0 1
14 -2 0 1 2 0 0 1
12 -1 0 2 3 0 0 1
13 1 0 4 4 0 0 1
11 2 0 2 1 0 0 2
14 -2 0 1 2 0 0 2
12 -1 0 2 3 0 0 2
13 1 0 3 4 0 0 2
0 0 0 0 0 0 0 0
34 21 2 1 5 0 0 2
-1 1 -1 1 1 2 0 0
35 21 2 2 5 0 0 1
-1 1 -1 2 1 1 0 0
0 0 0 0 0 0 0 0
2 -1 0 1 1 0 0 0
-1 1 -1 2 2 4 0 0
2 -1 0 2 1 0 0 0
-1 1 -1 1 2 3 0 0
0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0
```

```
integer, parameter :: ovm_LOAD_U = 11
integer, parameter :: ovm_LOAD_UBAR = 12
integer, parameter :: ovm_LOAD_V = 13
integer, parameter :: ovm_LOAD_VBAR = 14
integer, parameter :: ovm_LOAD_VECTOR = 15
integer, parameter :: ovm_LOAD_CONJ_VECTOR = 16

integer, parameter :: ovm_ADD_MOMENTA = 1
integer, parameter :: ovm_CALC_BRAKET = 2

integer, parameter :: ovm_PROPAGATE_PSI = 31
integer, parameter :: ovm_PROPAGATE_PSIBAR = 32
integer, parameter :: ovm_PROPAGATE_UNITARITY = 33
integer, parameter :: ovm_PROPAGATE_FEYNMAN = 34
integer, parameter :: ovm_PROPAGATE_COL_FEYNMAN = 35

integer, parameter :: ovm_FUSE_VEC_PSIBAR_PSI = -1
integer, parameter :: ovm_FUSE_PSI_VEC_PSI = -2
integer, parameter :: ovm_FUSE_PSIBAR_PSIBAR_VEC = -3
integer, parameter :: ovm_FUSE_GLU_GLU_GLU = -4
integer, parameter :: ovm_FUSE_WFS_V4 = -5
```