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NON-OVERLAPPING DOMAIN DECOMPOSITION METHOD AND NON-LINEAR DIFFUSION ACCELERATION IN THE FRAMEWORK OF THE IDT TRANSPORT SOLVER OF THE APOLLO3 CODE

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Paris 7/12/2018



- 1. IDT with HCC: the Integro-Differential Transport (IDT) solver with Heterogeneous Cartesian Cells (HCC)
- 2. Spatial integration
- 3. Non-linear diffusion iterations & parallelism
- 4. 3D results on workstation and mid-range HPC (Callisto)



IDT with HCC

HETEROGENEOUS CARTESIAN CELLS (HCC)



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3D MODELIZATION OF THE PIN CELL

Full 3D pin cell

piecewise extruded geometry



Thermo-mechanical deformations (swelling + bowing)





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SPATIAL EXPANSION AND SOLUTION

$$\psi(\mathbf{r}, \mathbf{\Omega}) = e^{-\tau(0,l)}\psi^{-}(\mathbf{r}^{-}, \mathbf{\Omega}) + \int_{0}^{l} dx \ e^{-\tau(x,l)}q(\mathbf{r}^{-} + x\mathbf{\Omega}, \mathbf{\Omega})$$



Polynomial expansion for the source (linear)

Polynomial expansion for the interface angular flux up to the bilinear order

$$V_{\alpha}\overrightarrow{\psi}_{\alpha}(\Omega) = \sum_{s'\in x, y, z} I_{\alpha, s'}(\Omega)\overrightarrow{\psi}_{s'}^{-}(\Omega) + \sum_{\beta\in c} C_{\alpha\beta}(\Omega)\overrightarrow{q}_{\beta}(\Omega), \ \alpha = 1, N_{R}$$
$$\gamma_{s}(\Omega)\overrightarrow{\psi}_{s}^{+}(\Omega) = \sum_{s'\in x, y, z} T_{s, s'}(\Omega)\overrightarrow{\psi}_{s'}^{-}(\Omega) + \sum_{\alpha\in c} E_{s, \alpha}(\Omega)\overrightarrow{q}_{\alpha}(\Omega), \ s \in x, y, z$$

HCC COEFFICIENTS

The integral transport equation is used to generate the equations for both volume and surface spatial moments. The numerical integration (analytically along the trajectory) based on <u>local projections of the geometrical discontinuities.</u> Trajectories are distributed along each interval using Gauss-Legendre quadrature along each transverse interval.

$$\int_{V\alpha} d\mathbf{r} f(\mathbf{r}) \simeq \sum_{t'//\Omega_{xy} t' \cap D_{\alpha,xy}} w_{xy,t'} \sum_{t//\Omega t \cap D_{\alpha}} w_{sz,t}^{t'} \int_{l_{\alpha,t}^{-}}^{l_{\alpha,t}^{+}} dl f(\mathbf{r}_{s,t',t} + l\mathbf{\Omega})$$



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ANALYTICAL INTEGRATION ON THE 3D SLICES



ISOPARAMETRIC LINEAR TRANSFORMATION



Linear transformation of the spatial coordinates

$$\mathbf{r} = \mathbf{r}_0 + [\mathbf{r_1} - \mathbf{r_0}, \mathbf{r_2} - \mathbf{r_1}] \mathbf{u}$$

Linear transformation of the base

$$\begin{cases} 1 \\ \mathbf{r} \end{cases} = \begin{cases} 1 \\ \mathbf{r}_0 \end{cases} + \begin{bmatrix} 1 & 0 \\ \mathbf{r_1} - \mathbf{r_0} & \mathbf{r_2} - \mathbf{r_1} \end{bmatrix} \begin{cases} 1 \\ \mathbf{u} \end{cases}$$

$$\mathbf{u} = \{x, y\}$$

$$y = x \quad \text{for triangle}$$

$$y = 1 - x \quad \text{for inverse triangle}$$

$$y = 1 \quad \text{for slice}$$

$$x \in [0, 1]$$

$$x \wedge I = \begin{bmatrix} x, y \\ y = 1 \\ y = 1 \end{bmatrix}$$

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 \xrightarrow{v}

ELEMENTARY SLICE AND EXPONENTIAL INTEGRAL FUNCTIONS



OPTIMIZATION OF COEFFICIENT CALCULATION

■ 8 seed functions, 6 for parallelograms and triangles and 2 for double-triangle slice

$$\{K_2(\tau_{\max}), K_{0,2}(\tau_{\max}), \dots, K_{0,0,0,0,0,2}(\tau_{\max})\}$$
$$\{L_{1,2}(\tau_{1,\max}, \tau_{2,\max}), L_{2,1}(\tau_{1,\max}, \tau_{2,\max})\}$$

Linear expansion of transport matrix coefficient

$$\frac{d\psi}{d\Sigma}(x,\Sigma) = -x\psi(x,\Sigma) + \int_0^x dy \ yq(y)e^{-\Sigma(x-y)}$$

Linear expansion of the matrix coefficients $\overrightarrow{\Sigma}_{cell} = \{\Sigma_{\gamma}\}_{\gamma \in cell}$ $C_{\alpha,\beta}(\overrightarrow{\Sigma}_{cell}) = C_{\alpha,\beta}(\overrightarrow{\Sigma}_{0}) + \sum_{\gamma \in cell} \frac{\partial C_{\alpha,\beta}}{\partial \Sigma_{\gamma}}(\overrightarrow{\Sigma}_{0})(\Sigma_{\gamma} - \Sigma_{\gamma,0}) + o(\Delta\Sigma^{2})$ $\overrightarrow{\Sigma}_{cell} \in [1 - \delta, 1 + \delta] \times \overrightarrow{\Sigma}_{0}$ $\delta = \sqrt{5 \text{ pcm}} \simeq 0,0071$



Domain

Decomposition

Method (DDM)

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Global eigenvalue problem : $x \equiv (\mathbf{r}, \mathbf{\Omega}, E) \in X$

$$(L-H)\psi(x) = \frac{1}{\lambda}F\psi(x) \qquad x \in X,$$

$$\psi^{-}(x) = 0 \qquad x \in \partial X^{-}.$$

DD boundary-value problems (PBJ) :

$$\begin{bmatrix} (L-H)_{\alpha} & 0\\ 0 & (L-H)_{\beta} \end{bmatrix} \begin{bmatrix} \psi_{\alpha}\\ \psi_{\beta} \end{bmatrix}^{(n+1)} = \begin{bmatrix} q_{\alpha}\\ q_{\beta} \end{bmatrix}^{(n)} + \begin{bmatrix} 0 & \delta(x-x_{\alpha\leftarrow\beta}^{-})\\ \delta(x-x_{\beta\leftarrow\alpha}^{-}) & 0 \end{bmatrix} \begin{bmatrix} \psi_{\alpha}^{+}\\ \psi_{\beta}^{+} \end{bmatrix}^{(n)}$$

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DDM PREFORMACES

The non-overlapping DDM+PI is less effective than the standard Sn iterative scheme. (Gauss-Jacobi vs. Gauss-Seidel)

The DDM suffers from oscillatory convergence behavior. The effect is accentuated as the number of subdomains increases.



Basic pattern B A

В

B A

С

С

4-subdomain DD

С	В	Α	С	С	С
С	В	A	В	В	В
С	В	Α	Α	А	А
А	Α	Α	А	В	С
В	В	В	Α	В	С
С	С	С	Α	В	С

С В В С С А В В Β C Β В С В В Β A A B С В A A В В A A C А В B В В В В В B A C C A С C A В С С С С В C A В В С С С С С А С С A В В В В C Β A Β С Β A В В В А A A A С A A Α Α А В С А А В C A A A A В В В В В В В B А С С A С С С В С В C C

16-subdomain DD

Spectral radius on the fission integral

$$\rho = \frac{\left|I_{fis}^{(e)} - I_{fis}^{(e-1)}\right|}{\left|I_{fis}^{(e-1)} - I_{fis}^{(e-2)}\right|}, \qquad I_{fis}^{(e)} = \sum_{\forall r} \sum_{is \in r} \sum_{g}^{N_g} \left(\nu \Sigma_f\right)_{is}^g \phi_{r,g}^{(e)}(r)$$

Number of power iterations

$$N_e \sim \frac{\ln(2)}{\ln(2)}$$
,

Spectral radius vs. n. of subdomains

Algorithm N. of subdomains	Dire	ect	PBJ	M
	ρ	N _e	ρ	N _e
3 x 3	0.818	58	0.941	190
6 x 6	0.818	58	0.946	208
9 x 9	0.818	58	0.948	216

 \Rightarrow Ineffective, needs acceleration !



Non-linear diffusion: Coarse Mesh Finite Difference (CMFD)
 In this case the non-linear operator is an acceleration operator for DDM transport iterations.

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NON-OVERLAPPING DDM + NON-LINEAR DIFFUSION

Coarse phase space: energy, space and angle

$$y \equiv \int_y dx \in Y$$

$$\begin{split} (\nabla \cdot J + \Sigma_T \phi)(y) &= H_0 \phi(y) + \frac{F \phi(y)}{\lambda}, & \forall \ y \in Y, \\ \text{Modified Fick's Low} \rightarrow & J(y) &= -\frac{p}{\Sigma_T} \nabla \phi(y) + \nu_T \phi(y), \\ & J(y) &= \beta_T \phi(y), & \forall \ y \in \partial Y. \end{split}$$

Equivalence parameter (transport-computed drift velocity)

$$\nu_T(y) = \left[\frac{\int_y dx \left[J_\alpha^{(n+\frac{1}{2})} + \frac{p}{\Sigma_\alpha} \nabla \cdot \phi_\alpha^{(n+\frac{1}{2})} \right](x)}{\int_y dx \ \phi_\alpha^{(n+\frac{1}{2})}(x)} \right]_T$$

EQUIVALENCE + STABILITY + CORRECTION

Equivalence

$$\psi_{\alpha}^{+(n+1)}(x) = \psi_{\alpha}^{+(n+\frac{1}{2})}(x) \frac{\phi(y)}{\int_{y} dx \ \phi_{\alpha}^{(n+\frac{1}{2})}(x)} x \in \partial X_{\alpha}$$

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SPECTRAL RADIUS OF VARIOUS ACCERLERATION METHODS





- The spectral radius source iterations (SI) is bounded by the scattering ratio "c", i.e. the ratio among the scattering and total cross sections, (in nuclear reactors c ~ 1)
- □ The CMFD guarantees a huge reduction of the # of DoF for the acceleration operator.

SINGLE PROCESSOR « STRONG SCALING » TEST (1) : CMFD EFFICIENCY ON THE 3X3 COLORSET



- The CMFD guarantees a DDM range with no loss in performances w.r.t. the direct calculation!
- Limit : performances deteriorate for subdomains having # of cells < 6x6 pin cells per assembly</p>
- Advances: the fuel assembly seems an optimal compromise for the subdomain size.

SINGLE PROCESSOR TEST (1) : CACHE EFFECT



$$S = E = \frac{T(1)}{T(n_{sub})}$$

 \square # of outer iterations = 10

- □ # of iterations for outer CMFD = 10
- □ # of inner transport iterations = 10
- □ # of iterations for inner CMFD= 10

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DOMAIN RECONSTRUCTION





← Hetrogeneous Cartesian cell

← Generating Calculation Units (GCU)

geometries



← PIVOT geometry (ECU) (reactor core)

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DDM +CMFD IN THE IDT SOLVER



IDT HYBRID PARALLELISM ARCHITECTURE

Distribution of the Subdomains (GCU) on the MPI procress



4 subdomains

Present limit: CMFD runs on single MPI process (W. FORD PhD in progress to solve such an issue)





DISTRIBUTED/SHARED-MEMORY PARALLEISM

Initial guess, DO loop, iterate until convergence: MPI Comm. : update of the interface flux (b.c. for the subdomains)

!OMP PARALLEL

for each $\alpha \in N(MPI)$ do :

load incoming flux, compute subdomain α , homogenize

!OMP END PARALLEL

MPI Comm. : gather on 1 single MPI data to feed CMFD Solve CMFD operator (inner **!OMP PARALLEL**)

MPI Comm. : scatter the CMFD flux and eigenvalue to all processes **!OMP PARALLEL**

for each $\alpha \in N(MPI)$ do : transport flux update by CMFD acceleration

+ fission source update + eigenvalue (from CMFD)

!OMP END PARALLEL

Convergence test: eigenvalue, fission source (isotope-wise), flux angular moments, interface angular flux

End loop



3D Results*





VERA (CASL) BENCHMARK : WATTS BAR UNIT 1 COLORSET

- More than 13000 materials, 47-group P3 XS library
- ~8000 different pins cells (self shielded-depleted materials)
- Million spatial mesh, 160 directions, 16 angular moments, 4 spatial moments (linear Short Characteristics)
- □ 4-4-2 surface submesh + CMFD at the pin-cell level
- □ 3 x 3 x 32 = 228 subdomains



* pcm = pour cent mile

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AXIAL POWER ERROR DISTRIBUTION



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COMPUTATIONAL TIME

Elapsed Time	OpenMP (20 threads)	MPI/OpenMP (20 nodes, 12 threads/node 240 threads)	
MOSC	24h (99%) (gfortran)	1h40 (96%)	
	18h (99%) (Intel)	(gfortran)	
CMFD	1min (<0.1%)	1min (<1%)	
Flux Exchange & misc.	<1min	6min (4%)	
Transport + CMFD # of iterations	8	8	
Total	24h30 / 18h15	1h45	ige 3



3D 3x3 Colorset 281Gr XS library (P3)

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3D COLORSET



1,535,600 regions (110 Z steps) 281 groups, 16 angular moments (P3) 198 (3x3x22) subdomains ~ 1 Tbyte of DoF





Radial distribution

Relative pin power error vs. TRIPOLI4

Taux de fission crayon intégré axialement



Code-to-code Comparison between nTRACER and the stand-alone IDT solver of APOLLO3 Young Suk Ban^{*1)}, Emiliano Masiello²⁾, Roland Lenain²⁾, Han Gyu Joo¹⁾ and Richard Sanchez^{1) 2),} Nuclear Science and Engineering (to be published).

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Cea 3D COLORSET : AXIAL POWER

Distribution axiale du taux de fission intégrée par assemblage (Maquette)





	k-eff	Dr	R.M.S.	MAX.	
TRIPOLI-4	1.05575	(reference, std. 0.6 pcm*)			
IDT	1.05437	-138 pcm	0.36 %	1.39 %	



Elapsed Time	OpenMP (20 threads)	MPI/OpenMP (20 nodes, 12 threads/node 240 threads)
	Time	Time
MOSC	24.4h	1.7h
CMFD	0.5h (2%)	0.5h (26%)
Flux Exchange & misc.	6sec. (<1%)	6min. (4%)
Transport + CMFD # of iterations	18	18
Total	24.9h	2.2h



3D FULL CORE

Cer EOLE (UH1.2) 3D CORE SIMULATION WITH APOLLO3





- 164 796 regions
- 62 092 cartesian cells (CMFD mesh)
- S12 C-L quadrature = 288 direction
- 281-group P1 XS library (4 angular moments)
- 3-3-1 surface mesh,
- for a total of 33 GB

Pascal ARCHIER, Bastien FAURE, Jean-Marc PALAU, Jean-François VIDAL, Emiliano MASIELLO, DER/SPRC/LEPh 18-221





Elapsed Time	OpenMP (24 threads)	MPI/OpenMP (20 nodes, 12 threads/node 240 threads)
	Time	Time
MOSC	14h (85%)	40 min (21%)
CMFD	2h (15%)	2h (71%)
Flux Exchange & misc.	6sec. (25, <1%)	6min. (25, 4%)
Transport + CMFD # of iterations	15	15
Total	14.9h	2h45

A3 VS. T4 VS. EXPERIMENTAL FISSION DISTRIBUTION MESUREMENT



Pascal ARCHIER, Bastien FAURE, Jean-Marc PALAU, Jean-François VIDAL, Emiliano MASIELLO, DER/SPRC/LEPh 18-221

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AXIAL POWER DISTRIBUTION AND REACTIVITY



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RADIAL POWER DISTRIBUTION

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- 19x19 assembly-sized subdomains

- 264 pins/assembly
- 1.5 22 axial planes
 - about 10 radial regions/pellet
 = ~ 10 Millions of regions
 - 26 groups
- P3 (16 angular moments)
 - Linear MOSC (4 spatial moments)

= ~ 30 Billions of unknowns

784 GBYTES OF MEMORY: 1% COF, 84% TRA, 16% CMFD ~30 GBYTES/NODE

ACCURACY (NTRACER VS. IDT)



Axial Layer

	k-eff	Reactivity error (pcm)	R.M.S.	MAX (%)
nTRACER-MC*	1.01505	-	-	-
nTRACER	1.01527	22	0.66	2.41
IDT(3-3-2)	1.01521	15	1.17	3.61
IDT(1-1-1)	1.01490	-15	0.46	2.40

* nTRACER-MC is a multigroup Monte Carlo solver, with Pn scattering expansion: it is not properly a reference !



PERORMANCES

12/ threads per node * 28 nodes = 336 threads Xeon L5640 2.26 GHz 36 Go / Node (CALLISTO-PLUTON) compiler gfortran + mpich

	Time		
	(3-3-2)	(1-1-1)	
TRANSPORT	55%	37%	
CMFD	44%	62%	
(Transport + CMFD iterations)	40	24	
Flux Exchange & misc.	<1	%	
Total	5h32	2h20	



Thank you!



FIRST CONCLUSION

□ The distributed-memory parallelism is mandatory for high-fidelity 3D full-

core transport simulations !

IDT Short-term updates in APOLLO3:

- Hybrid MPI/Open MP parallelism by the Domain Decomposition Method.*
- HCC with unstructured volume sub mesh.
- Hybrid MPI/Open MP parallelism for the synthetic acceleration (CMFD) **

* R.LENAIN, E. MASIELLO, F. DAMIAN, R. SANCHEZ, "Domain Decomposition Method for 2d and 3d Transport Calculations Using Hybrid Mpi/Openmp Parallelism," M&C 2015, Nashville TN

Long-term updates:

- Triangular and tetrahedral mesh.

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WEAK SCALABILITY



- □ Assembly-sized subdomains
- □ 1 to 24 subdomains (and threads)
- Processors run from 1 to 12
- The hyperthreading is switched-on from 13 to 24

$$n_{threads} = n_{sub}$$

$$S = \frac{n_{thread} * T(1)}{T(n_{thread})}$$

$$E = \frac{S}{n_{thread}}$$

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	9x9 cluster (DDM with 81 assembly-sized subdomains)				
	CMFD (1x1, 281grp)	CMFD (4x4, 26grp)	DDM+CMFD (4X4, 26grp)	DDM+CMFD (4X4, 26grp)	
# of subdomains	1	1	81	81	
# of processors	1	1	1	12	
Computational time (s)	229398 (63h)	20562 (5h30)	19395 (5h30)	1735 (29min)	
<i># of outer iterations</i>	9	11	13	13	
<i># of transport iterations</i>	5053	8090	7740	7740	
# of CMFD outer iterations	98	57	260	232	

- 81 assemblies, 281 groups, P1 scattering, 40 directions, ~150000 regions, ~ 100000 sets of XS (~ 10Gb.)
- □ the colorset does not have internal symmetry.

3D Core simulation:

- 193 assemblies
- 264 pins/assembly
- 200 axial pellet/pin
- 10 radial regions/pellet
- 400 nuclides per regions
- 5 reaction per nuclide
- 10 Kbytes/reactions



=~ 2 000 T-bytes of data

HYBRID MPI/OPENMP PARALLELISM

Points	OpenMP	MPI	Hybrid OpenMP/MPI
Available Memory	-	++	++
# of processors	-	++	++
CMFD communications	++	-	+
Load balance	++	-	+
Memory efficiency	++	-	+

- \Rightarrow More than 1 subdomains on a single MPI process
- ⇒ OpenMP paradigms applied to the subdomains sharing the same MPI process.
- \Rightarrow The iterative algorithm remains unchanged !