Reconciling mathematics with programming for developing sustainable HPC codes in continuum mechanics

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TUDelft

Continuum Mechanics

Fluids:

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla P + \nabla \cdot \mathbf{S} + \rho g$$

Solids:

$$\rho \frac{\partial^2 \mathbf{x}}{\partial t^2} = \nabla \cdot \mathbf{S} + \mathbf{F}$$

code_aster FLUENT OpenFOAM STAR-CCM+ ReFRESCO SIMULIA ABAQUS

Basic Linear Algebra Subroutines

Level 1 BLAS

dim scalar vector vector scalars 5-element array		prefixes
SUBROUTINE xROTG (A, B, C, S)	Generate plane rotation	S, D
SUBROUTINE xROTMG(D1, D2, A, B, PARAM)	Generate modified plane rotation	S, D
SUBROUTINE xROT (N, X, INCX, Y, INCY, C, S)	Apply plane rotation	S, D
SUBROUTINE xROTM (N, X, INCX, Y, INCY, PARAM)	Apply modified plane rotation	S, D
SUBROUTINE xSWAP (N, X, INCX, Y, INCY)	$x \leftrightarrow y$	S, D, C, Z
SUBROUTINE xSCAL (N, ALPHA, X, INCX)	$x \leftarrow \alpha x$	S, D, C, Z, CS, ZD
SUBROUTINE xCOPY (N, X, INCX, Y, INCY)	$y \leftarrow x$	S, D, C, Z
SUBROUTINE xAXPY (N, ALPHA, X, INCX, Y, INCY)	$y \leftarrow \alpha x + y$	S, D, C, Z
FUNCTION xDOT (N, X, INCX, Y, INCY)	$dot \leftarrow x^T y$	S, D, DS
FUNCTION xDOTU (N, X, INCX, Y, INCY)	$dot \leftarrow x^T y$	C, Z
FUNCTION xDOTC (N, X, INCX, Y, INCY)	$dot \leftarrow x^H y$	C, Z
FUNCTION xxDOT (N, X, INCX, Y, INCY)	$dot \leftarrow \alpha + x^T y$	SDS
FUNCTION xNRM2 (N, X, INCX)	$nrm2 \leftarrow \lVert x \rVert_2$	S, D, SC, DZ
FUNCTION xASUM (N, X, INCX)	$asum \leftarrow \lVert re(x) \rVert_1 + \lVert im(x) \rVert_1$	S, D, SC, DZ
FUNCTION IxAMAX(N, X, INCX)	$amax \leftarrow 1^{st} k \ni \lvert re(x_k)\rvert + \lvert im(x_k)\rvert = max(\lvert re(x_i)\rvert + \lvert im(x_i)\rvert)$	S, D, C, Z

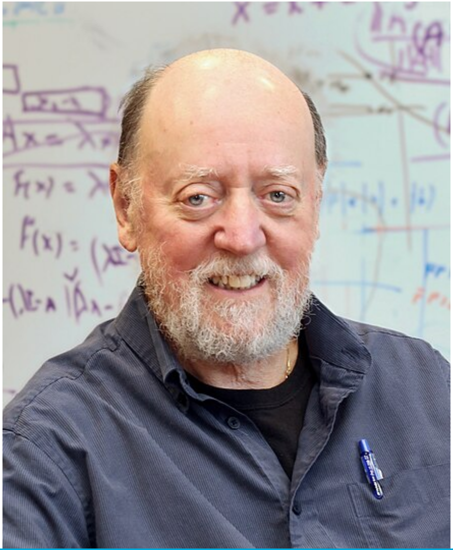
Level 2 BLAS

options dim b-width scalar matrix vector scalar vector		
xGEMV (TRANS, M, N, ALPHA, A, LDA, X, INCX, BETA, Y, INCY)	$y \leftarrow \alpha Ax + \beta y, y \leftarrow \alpha A^T x + \beta y, y \leftarrow \alpha A^H x + \beta y, A - m \times n$	S, D, C, Z
xGBMV (TRANS, M, N, KL, KU, ALPHA, A, LDA, X, INCX, BETA, Y, INCY)	$y \leftarrow \alpha Ax + \beta y, y \leftarrow \alpha A^T x + \beta y, y \leftarrow \alpha A^H x + \beta y, A - m \times n$	S, D, C, Z
xHEMV (UPLO, N, ALPHA, A, LDA, X, INCX, BETA, Y, INCY)	$y \leftarrow \alpha Ax + \beta y$	C, Z
xHBMV (UPLO, N, K, ALPHA, A, LDA, X, INCX, BETA, Y, INCY)	$y \leftarrow \alpha Ax + \beta y$	C, Z
xHPMV (UPLO, N, ALPHA, AP, X, INCX, BETA, Y, INCY)	$y \leftarrow \alpha Ax + \beta y$	C, Z
xSYMV (UPLO, N, ALPHA, A, LDA, X, INCX, BETA, Y, INCY)	$y \leftarrow \alpha Ax + \beta y$	S, D
xSBMV (UPLO, N, K, ALPHA, A, LDA, X, INCX, BETA, Y, INCY)	$y \leftarrow \alpha Ax + \beta y$	S, D
xSPMV (UPLO, N, ALPHA, AP, X, INCX, BETA, Y, INCY)	$y \leftarrow \alpha Ax + \beta y$	S, D
xTRMV (UPLO, TRANS, DIAG, N, A, LDA, X, INCX)	$x \leftarrow Ax, x \leftarrow A^T x, x \leftarrow A^H x$	S, D, C, Z
xTBMV (UPLO, TRANS, DIAG, N, K, A, LDA, X, INCX)	$x \leftarrow Ax, x \leftarrow A^T x, x \leftarrow A^H x$	S, D, C, Z
xTPMV (UPLO, TRANS, DIAG, N, AP, X, INCX)	$x \leftarrow Ax, x \leftarrow A^T x, x \leftarrow A^H x$	S, D, C, Z
xTRSV (UPLO, TRANS, DIAG, N, A, LDA, X, INCX)	$x \leftarrow A^{-1}x, x \leftarrow A^{-T}x, x \leftarrow A^{-H}x$	S, D, C, Z
xTBSV (UPLO, TRANS, DIAG, N, K, A, LDA, X, INCX)	$x \leftarrow A^{-1}x, x \leftarrow A^{-T}x, x \leftarrow A^{-H}x$	S, D, C, Z
xTPSV (UPLO, TRANS, DIAG, N, AP, X, INCX)	$x \leftarrow A^{-1}x, x \leftarrow A^{-T}x, x \leftarrow A^{-H}x$	S, D, C, Z
options dim scalar vector vector matrix		
xGER (M, N, ALPHA, X, INCX, Y, INCY, A, LDA)	$A \leftarrow \alpha xy^T + A, A - m \times n$	S, D
xGERU (M, N, ALPHA, X, INCX, Y, INCY, A, LDA)	$A \leftarrow \alpha xy^T + A, A - m \times n$	C, Z
xGERC (M, N, ALPHA, X, INCX, Y, INCY, A, LDA)	$A \leftarrow \alpha xy^H + A, A - m \times n$	C, Z
xHER (UPLO, N, ALPHA, X, INCX, A, LDA)	$A \leftarrow \alpha xx^H + A$	C, Z
xHPR (UPLO, N, ALPHA, X, INCX, AP)	$A \leftarrow \alpha xx^H + A$	C, Z
xHER2 (UPLO, N, ALPHA, X, INCX, Y, INCY, A, LDA)	$A \leftarrow \alpha xy^H + y(\alpha x)^H + A$	C, Z
xHPR2 (UPLO, N, ALPHA, X, INCX, Y, INCY, AP)	$A \leftarrow \alpha xy^H + y(\alpha x)^H + A$	C, Z
xSYR (UPLO, N, ALPHA, X, INCX, A, LDA)	$A \leftarrow \alpha xx^T + A$	S, D
xSPR (UPLO, N, ALPHA, X, INCX, AP)	$A \leftarrow \alpha xx^T + A$	S, D
xSYR2 (UPLO, N, ALPHA, X, INCX, Y, INCY, A, LDA)	$A \leftarrow \alpha xy^T + \alpha yx^T + A$	S, D
xSPR2 (UPLO, N, ALPHA, X, INCX, Y, INCY, AP)	$A \leftarrow \alpha xy^T + \alpha yx^T + A$	S, D

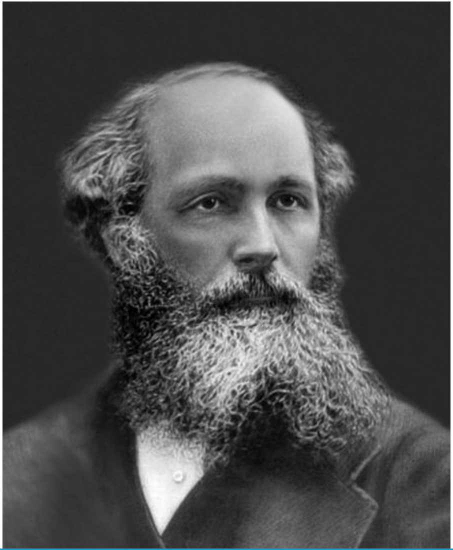
Level 3 BLAS

options dim scalar matrix matrix scalar matrix		
xGEMM (TRANSA, TRANSB, M, N, K, ALPHA, A, LDA, B, LDB, BETA, C, LDC)	$C \leftarrow \alpha op(A)op(B) + \beta C, op(X) = X, X^T, X^H, C - m \times n$	S, D, C, Z
xSYMM (SIDE, UPLO, M, N, ALPHA, A, LDA, B, LDB, BETA, C, LDC)	$C \leftarrow \alpha AB + \beta C, C \leftarrow \alpha BA + \beta C, C - m \times n, A = A^T$	S, D, C, Z
xHEMM (SIDE, UPLO, M, N, ALPHA, A, LDA, B, LDB, BETA, C, LDC)	$C \leftarrow \alpha AB + \beta C, C \leftarrow \alpha BA + \beta C, C - m \times n, A = A^H$	C, Z
xSYRK (UPLO, TRANS, N, K, ALPHA, A, LDA, BETA, C, LDC)	$C \leftarrow \alpha AA^T + \beta C, C \leftarrow \alpha A^T A + \beta C, C - n \times n$	S, D, C, Z
xHERK (UPLO, TRANS, N, K, ALPHA, A, LDA, BETA, C, LDC)	$C \leftarrow \alpha AA^H + \beta C, C \leftarrow \alpha A^H A + \beta C, C - n \times n$	C, Z
xSYR2K(UPLO, TRANS, N, K, ALPHA, A, LDA, B, LDB, BETA, C, LDC)	$C \leftarrow \alpha AB^T + \bar{\alpha} BA^T + \beta C, C \leftarrow \alpha A^T B + \bar{\alpha} B^T A + \beta C, C - n \times n$	S, D, C, Z
xHER2K(UPLO, TRANS, N, K, ALPHA, A, LDA, B, LDB, BETA, C, LDC)	$C \leftarrow \alpha AB^H + \bar{\alpha} BA^H + \beta C, C \leftarrow \alpha A^H B + \bar{\alpha} B^H A + \beta C, C - n \times n$	C, Z
xTRMM (SIDE, UPLO, TRANSA, DIAG, M, N, ALPHA, A, LDA, B, LDB)	$B \leftarrow \alpha op(A)B, B \leftarrow \alpha Bop(A), op(A) = A, A^T, A^H, B - m \times n$	S, D, C, Z
xTRSM (SIDE, UPLO, TRANSA, DIAG, M, N, ALPHA, A, LDA, B, LDB)	$B \leftarrow \alpha op(A^{-1})B, B \leftarrow \alpha Bop(A^{-1}), op(A) = A, A^T, A^H, B - m \times n$	S, D, C, Z

2



(Discrete) Vector Calculus



"it is evident that all analogies of this kind depend on principles of a more fundamental nature; and that [...] we should lose no time in availing ourselves of the mathematical labours of those who had already solved problems essentially the same"

J.C. Maxwell 1869

Challenge

Can we systematize the **computational and numerical** *aspects of computational mechanics?*

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- How to construct the discretizations?

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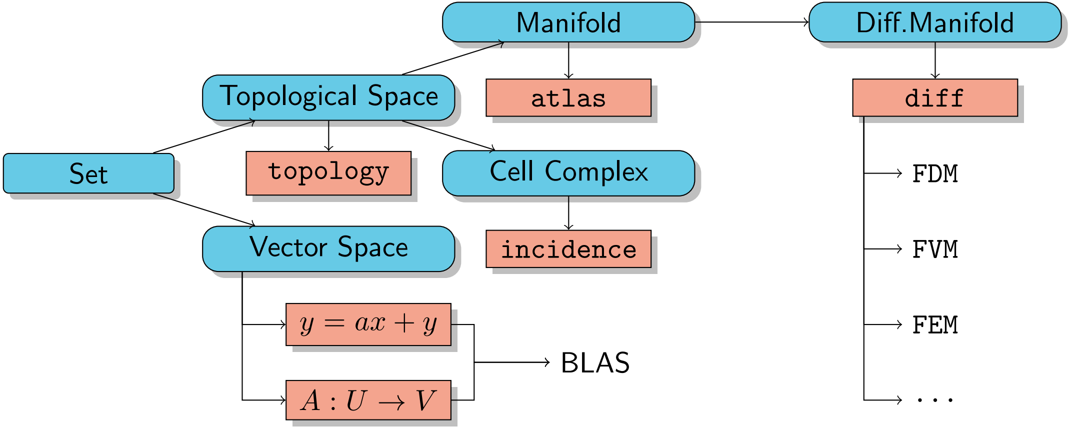
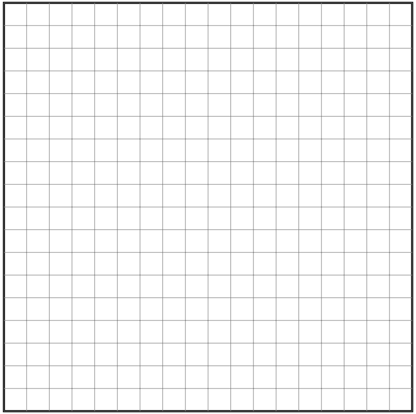
- How to construct the discretizations?

Set theory + OOP

Abstract Algebra

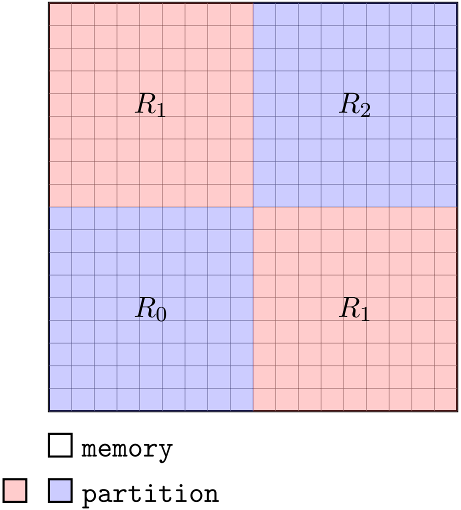


Partitions



☐ memory

Partitions

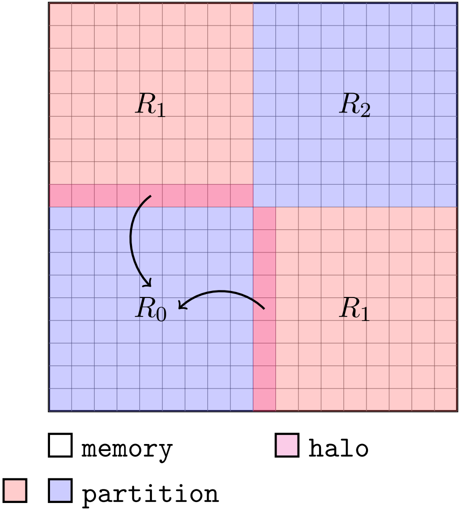


Definition

A partition P of a set X is a *collection of subsets* such that:

- $\emptyset \notin P$
- $\bigcup_i P_i = X$
- $P_i \cap P_j | i \neq j = \emptyset$

Partitions



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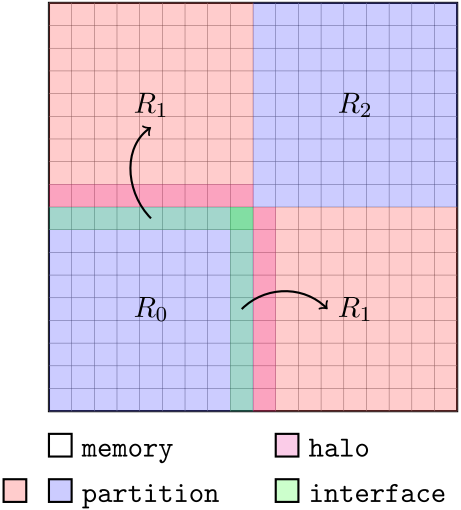

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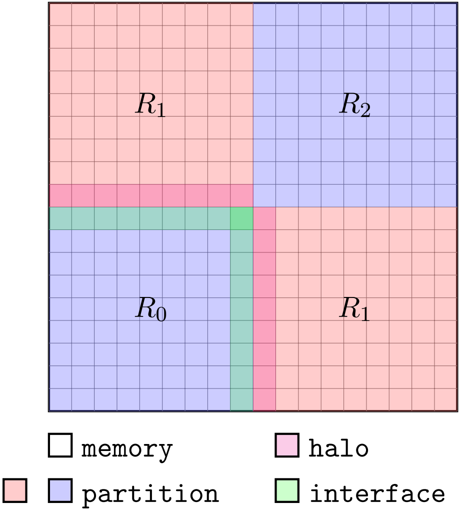
Partitions

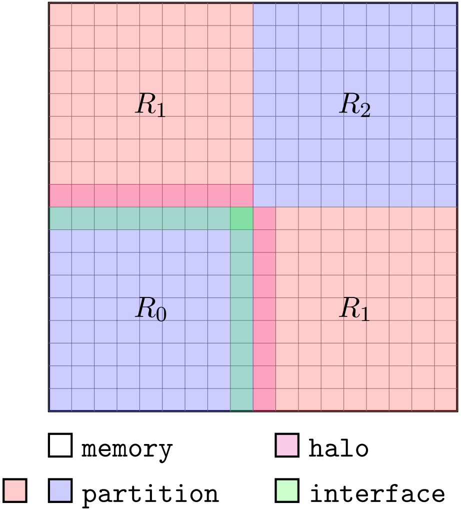


Definition

A cover C of a set X is a *collection of subsets* such that:

- $\emptyset \notin C$
- $\bigcup_i C_i \supset X$

Partitions



Definition

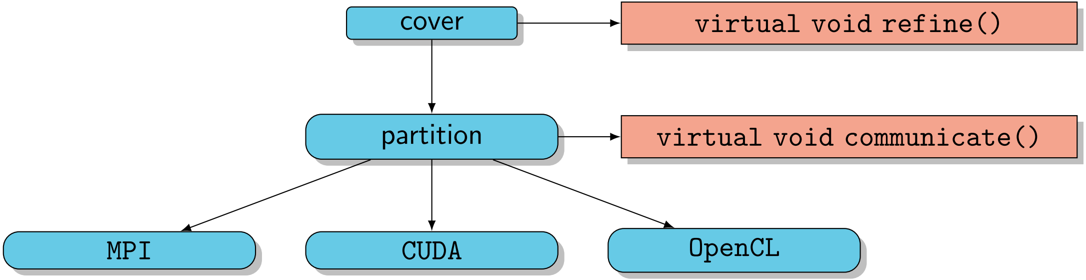
A cover C of a set X is a *collection of subsets* such that:

- $\emptyset \notin C$
- $\bigcup_i C_i \supset X$

Summary:

• set	X	`memory`
• partition	P	`MPI_comm`
• cover	C	`halo/interface`

Abstraction



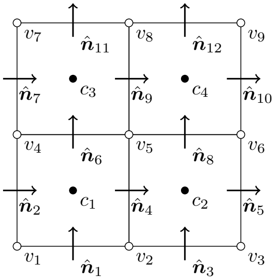
Mesh

What is a mesh?

Portability & Resilience

Why is it a challenge?

```
for(int i = 0; i < M; i++)
{
    ...
    for(int j = 0; j < N; j++)
    {
        ...
        y[i] = A[i][j] * x[i];
        ...
    }
    ...
}
```



Portability & Resilience

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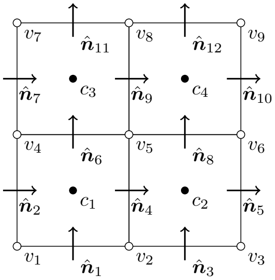
    }
    ...
}
```



Local memory accesses!

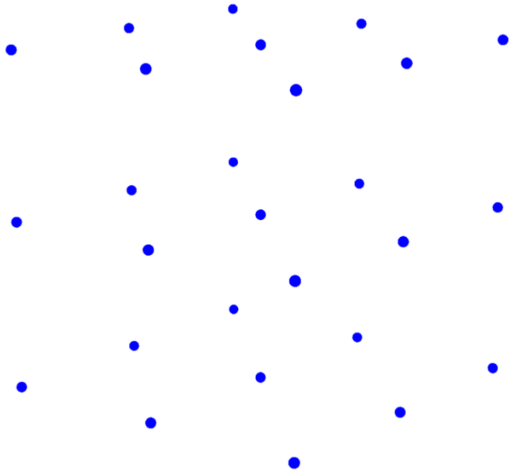
Connectivity - Cell complex

Connectivity - Cell complex

P

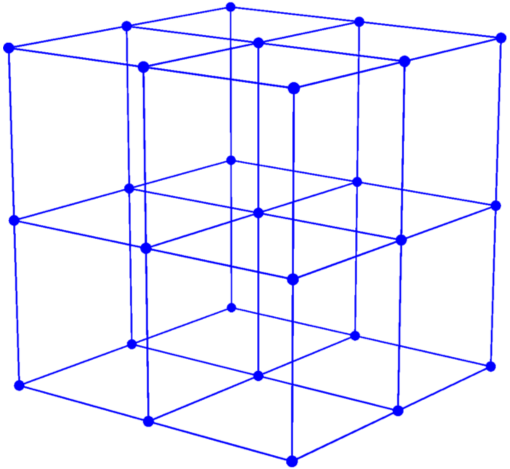
Connectivity - Cell complex

$$P \xrightarrow{E_0} L$$



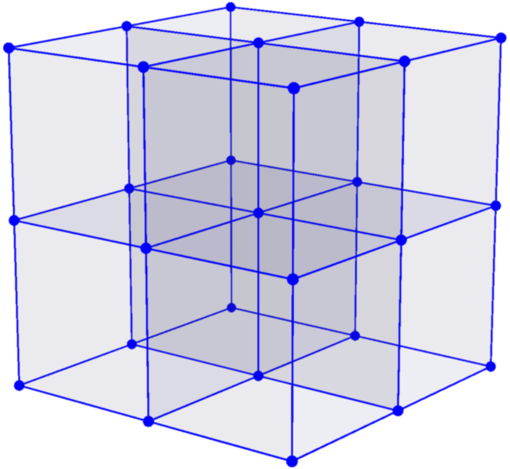
Connectivity - Cell complex

$$P \xrightarrow{E_0} L \xrightarrow{E_1} S$$



Connectivity - Cell complex

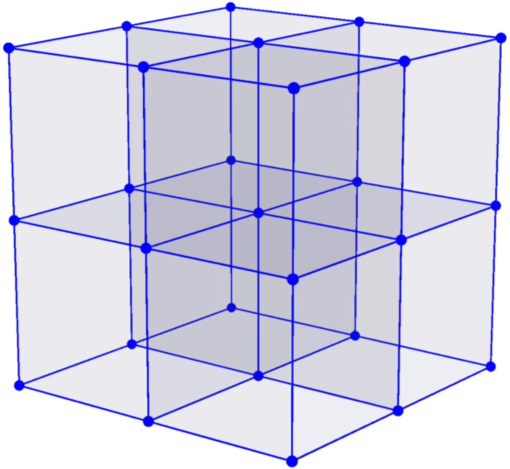
$$P \xrightarrow{E_0} L \xrightarrow{E_1} S \xrightarrow{E_2} V$$



Connectivity - Cell complex

co-chain

$$\boxed{P \xrightarrow{E_0} L \xrightarrow{E_1} S \xrightarrow{E_2} V}$$

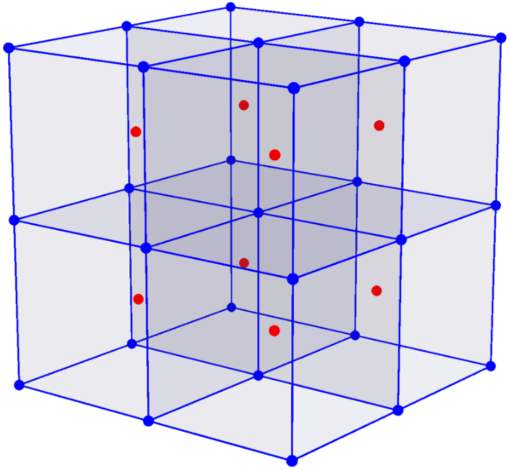


Connectivity - Cell complex

co-chain

$$\boxed{P \xrightarrow{E_0} L \xrightarrow{E_1} S \xrightarrow{E_2} V}$$

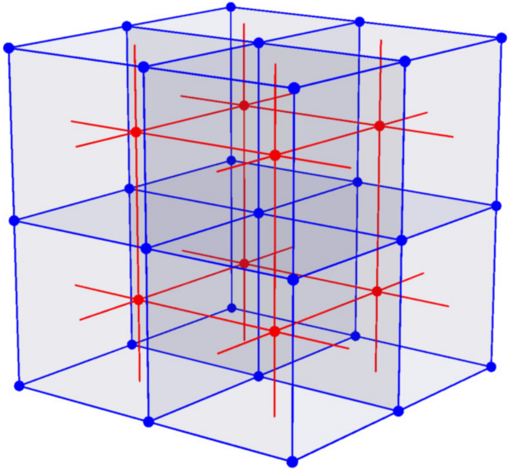
$$V \overset{\star}{\longleftrightarrow} \widetilde{P}$$



Connectivity - Cell complex

co-chain

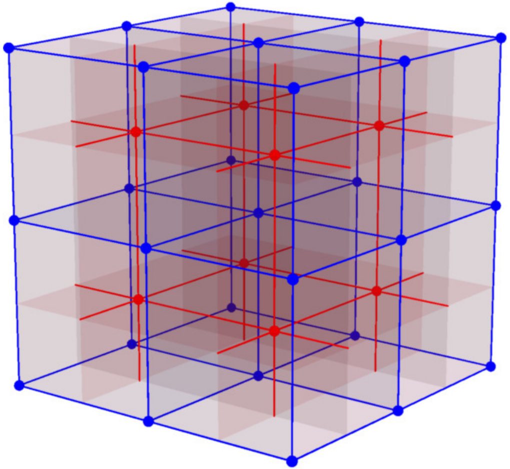
$$
\begin{tikzcd}
P \arrow[r, "E_0"] & L \arrow[r, "E_1"] & S \arrow[r, "E_2"] \arrow[d, leftrightarrow, "\star"] & V \arrow[d, leftrightarrow, "\star"] \\
 & & \widetilde{L} & \widetilde{P} \arrow[l, "\tilde{E}_0"']
\end{tikzcd}
$$



Connectivity - Cell complex

co-chain

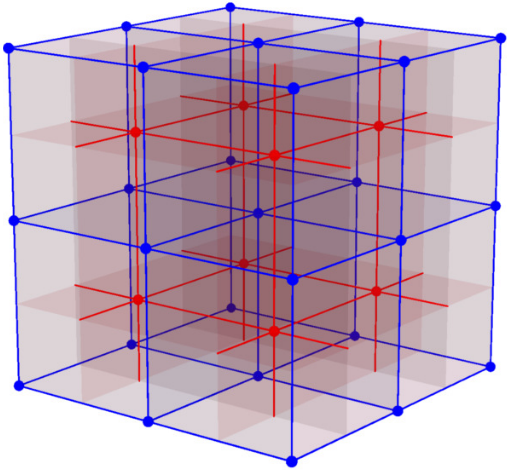
$$\begin{tikzcd}
P \arrow[r, "E_0"] & L \arrow[r, "E_1"] \arrow[d, leftrightarrow, "\star"] & S \arrow[r, "E_2"] \arrow[d, leftrightarrow, "\star"] & V \arrow[d, leftrightarrow, "\star"] \\
& \widetilde{S} & \widetilde{L} \arrow[l, "\tilde{E}_1"'] & \widetilde{P} \arrow[l, "\tilde{E}_0"']
\end{tikzcd}$$



Connectivity - Cell complex

co-chain

$$
\begin{tikzcd}
P \arrow[r, "E_0"] \arrow[d, leftrightarrow, "\star"] & L \arrow[r, "E_1"] \arrow[d, leftrightarrow, "\star"] & S \arrow[r, "E_2"] \arrow[d, leftrightarrow, "\star"] & V \arrow[d, leftrightarrow, "\star"] \\
\widetilde{V} & \widetilde{S} \arrow[l, "\tilde{E}_2"] & \widetilde{L} \arrow[l, "\tilde{E}_1"] & \widetilde{P} \arrow[l, "\tilde{E}_0"]
\end{tikzcd}
$$



Connectivity - Cell complex

co-chain

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\begin{tikzcd}
P \arrow[r, "E_0"] \arrow[d, leftrightarrow, "\star"] & L \arrow[r, "E_1"] \arrow[d, leftrightarrow, "\star"] & S \arrow[r, "E_2"] \arrow[d, leftrightarrow, "\star"] & V \arrow[d, leftrightarrow, "\star"] \\
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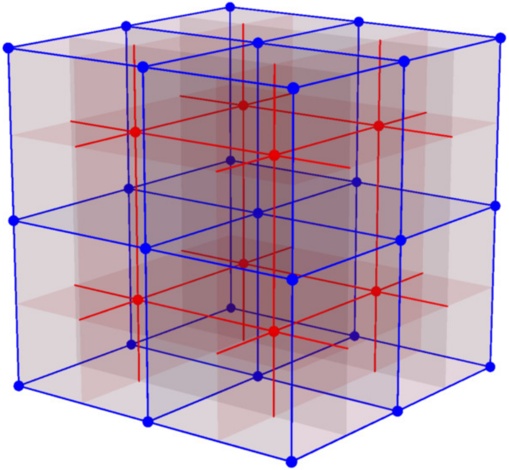
\end{tikzcd}
$$

chain



Connectivity - Cell complex

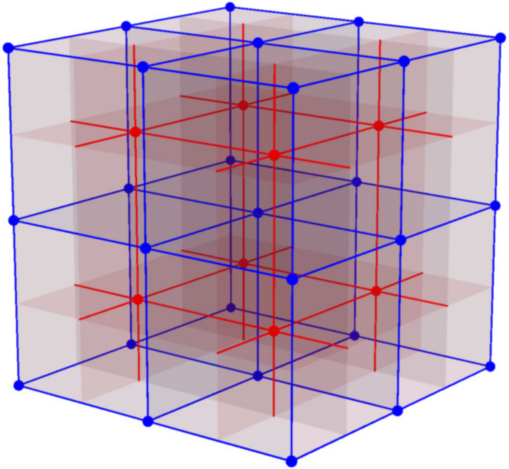
co-chain

$$
\begin{tikzcd}
P \arrow[r, "E_0"] \arrow[d, leftrightarrow, "\star"] & L \arrow[r, "E_1"] \arrow[d, leftrightarrow, "\star"] & S \arrow[r, "E_2"] \arrow[d, leftrightarrow, "\star"] & V \arrow[d, leftrightarrow, "\star"] \\
\widetilde{V} & \widetilde{S} \arrow[l, "\tilde{E}_2"'] & \widetilde{L} \arrow[l, "\tilde{E}_1"'] & \widetilde{P} \arrow[l, "\tilde{E}_0"']
\end{tikzcd}
$$

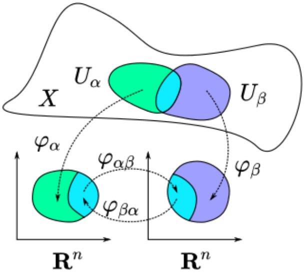
chain

Summary:

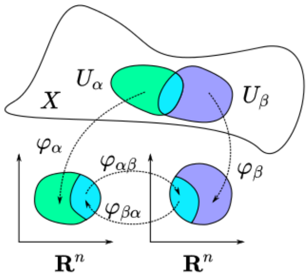
- C_i Cells!
- $E_i : C_i \to C_{i\pm1}$ Connectivity!



Coordinates - Manifold



Coordinates - Manifold

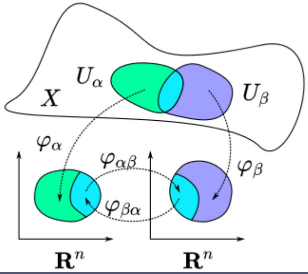


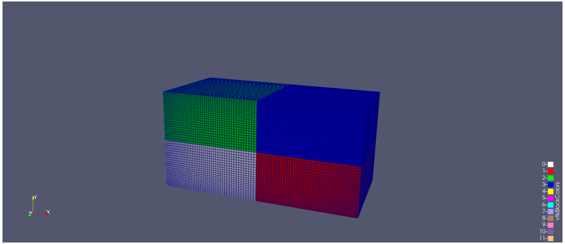
Definition

A manifold M is a topological space X equipped with a *collection of maps* φ that map to the Euclidean space $\mathbb{R}^n$.

$$\varphi_\alpha : U_\alpha \subseteq M \to \mathbb{R}^n$$

Coordinates - Manifold





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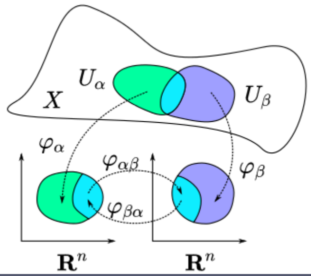

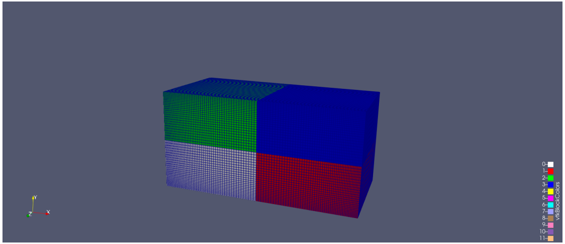

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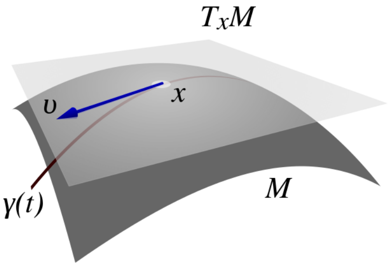
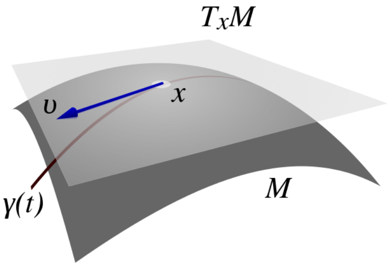
Summary:

- atlas φ `xdmf/vtk/etc`
- manifold M `mesh!`

Differentials - Differential Manifold



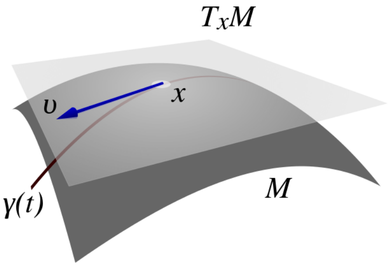
Differentials - Differential Manifold



Definition

A differential manifold M that is "smooth enough" to perform differentiation. This defines locally a tangent space T_xM.

Differentials - Differential Manifold



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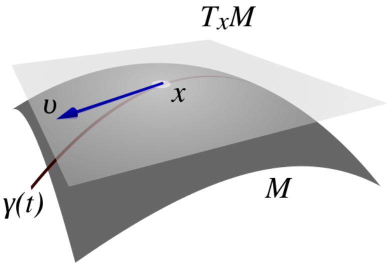
$$f \qquad f\,dl \qquad f\,dS \qquad f\,dv$$

$$\begin{array}{ccccccc}
\Lambda_0 & \xrightarrow{d} & \Lambda_1 & \xrightarrow{d} & \Lambda_2 & \xrightarrow{d} & \Lambda_3 \\
\downarrow \int & & \downarrow \int & & \downarrow \int & & \downarrow \int \\
P & \xrightarrow{E_0} & L & \xrightarrow{E_1} & S & \xrightarrow{E_2} & V
\end{array}$$

Differentials - Differential Manifold



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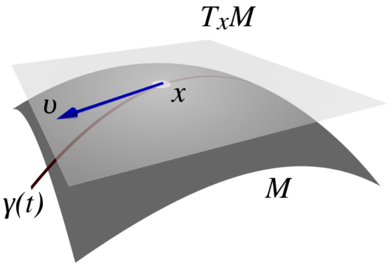

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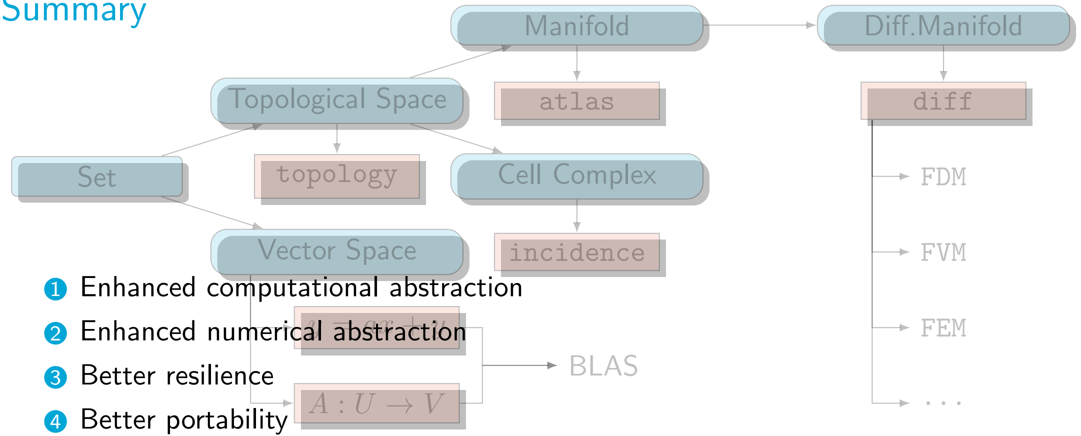
\end{array}
$$

Summary:

- Tangent Space T_xM `FDM/FVM/FEM/SEM`

Summary



1. Enhanced computational abstraction
2. Enhanced numerical abstraction
3. Better resilience
4. Better portability
5. Better interchangeability