University of Tuzla,
Faculty for Mechanical Engineering, Postgraduate study
Modelling, Simulation, Optimisation

Design Integration for Screw Compressors

Part 2:
Methods and Tools in Screw Compressor Design

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Methods and Tools in Screw compressor design

- **2-D design tools -** Conventional approach
  - **SCORPATH** (**S**crew **CO**mpressor **R**otor **P**rofiling **a**nd **TH**ermodynamics)
  - **2-D CAD Software: AutoCad, …**
- **3-D design tools -** More modern approach
  - **SCORPATH** (**S**crew **CO**mpressor **R**otor **P**rofiling **and TH**ermodynamics)
  - **3-D CAD** **MDT, Inventor, Catia, Solid Works, Pro Engineer**
  - **SCORG** (**S**crew **CO**mpressor **R**otor **G**rid)
  - **CCM (CFD)** **Comet, Star, CFX, Fluent …**
- **3-D design management -** Concurrent approach
  - **DISCO** (**D**esign **I**ntegration for **S**crew **CO**mpressors)

Mathematical model of continuum

Conservation laws: continuity, momentum, energy, concentration and space

$$\frac{d}{dt}\int_V \rho\phi dV + \int_S \rho\phi(\mathbf{v}-\mathbf{v}_s)\cdot d\mathbf{s} = \int_S \Gamma_\phi \operatorname{grad}\phi\cdot d\mathbf{s} + \int_S \mathbf{q}_{\phi S}\cdot ds + \int_V q_{\phi V}\cdot dV$$

	ϕ	Γ_ϕ	$\mathbf{q}_{\phi S}$	$q_{\phi V}$
Continuity	1	0	0	0
Fluid momentum	v_i	μ_{eff}	$\left[\mu_{eff}(\operatorname{grad}\mathbf{v})^{\mathrm{T}} - \left(\frac{2}{3}\mu_{eff}\operatorname{div}\mathbf{v}+p\right)\mathbf{I}\right]\cdot\mathbf{i}_i$	$f_{\mathrm{b},i}$
Solid momentum	$\frac{\partial u_i}{\partial t}$	η	$\left[\eta(\operatorname{grad}\mathbf{u})^{\mathrm{T}} + (\lambda\operatorname{div}\mathbf{u} - 3K\alpha\Delta T)\mathbf{I}\right]\cdot\mathbf{i}_i$	$f_{\mathrm{b},i}$
Energy	e	$\frac{k}{\partial e/\partial T}+\frac{\mu_t}{\sigma_T}$	$-\frac{k}{\partial e/\partial T}\frac{\partial e}{\partial p}\cdot\operatorname{grad}p$	T: grad v + h
Concentration	c_i	$\rho D_{i,\mathrm{eff}}$	0	s_{ci}
Space	$\frac{1}{\rho}$	0	0	0
Turbulent kinetic energy	K	$\mu+\frac{\mu_t}{\sigma_k}$	0	$P-\rho\varepsilon$
Dissipation	ε	$\mu+\frac{\mu_t}{\sigma_\varepsilon}$	0	$C_1 P\frac{\varepsilon}{k} - C_2\rho\frac{\varepsilon^2}{k} - C_3\rho\varepsilon\operatorname{div}\mathbf{v}$

$\rho=\rho(p,T),\quad e=e(p,T)$ Constitutive relations, equation of state and turbulence model.

Elements for successful CCM calculation

- Physically sound system
- Discretisation of PDE, space and time
- Regular numerical grid which describes a system well
- Well defined Initial and Boundary conditions
- Reliable and robust discretisation scheme
- A lot of computational resources and time

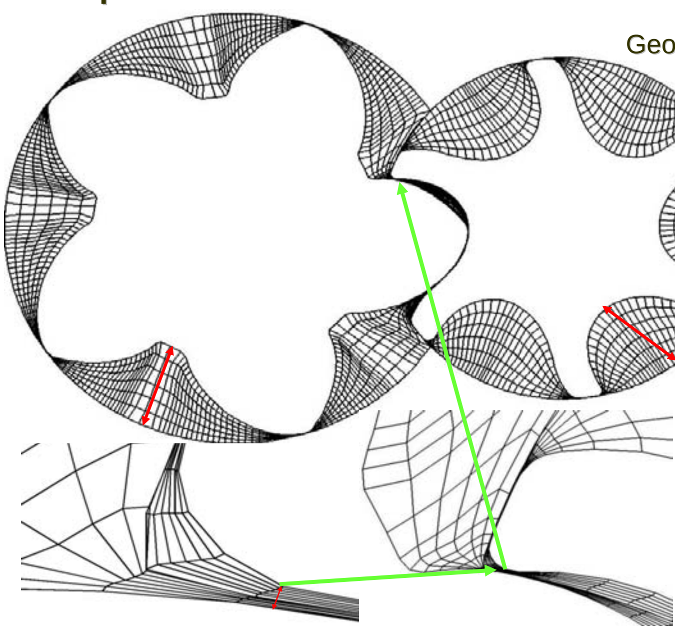
Computational Continuum Mechanics in Screw Compressors

- A commercial CCM solver(s) capable for efficient calculation
- "Expert system" for application in screw machines

- **METHODs:** Analytical Grid Generation & commercial numerical solver
  - Finite volume method, block-structured hexahedral mesh
  - Moving domains, sliding boundaries
  - Automatic running and analysis of the results

- **TOOLs:** ***SCORG*** - Analytical grid generation & Pre-processor
  COMET – Commercial CCM solver
  - Hermite transfinite interpolation with multidimensional stretching functions,
  - Boundary adaptation, smoothing, orthogonalisation and regularity check,
  - Fast and reliable calculation of thermodynamic properties of real fluids,
  - Multiphase flow, novel boundary conditions, mesh movement
  - Simultaneous generation and calculation of fluid/solid interaction
  - Automatic transfer to the CCM solver and Post-processing

Problems associated with numerical analysis and operation of Screw Machines



Geometry ratio 300-1000

Regions of highly turbulent flow and fully laminar flow

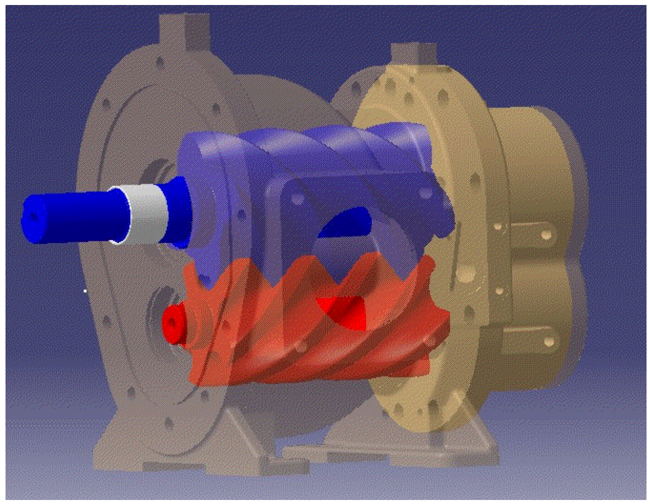
Transonic velocities

Large pressure gradients

High temperatures

Problems associated with numerical solution in screw machines

- Boundary conditions: Usually inlet - outlet, or pressure boundaries
- Refrigeration and other applications with real gasses
- Distortions in order of magnitude of the size of clearances
- Multiphase flows, multi-domain solutions



Boundary conditions

- Wall boundaries with wall functions are introduced on the housing and rotors.

- Compressor positioned between suction and discharge receivers of small volume

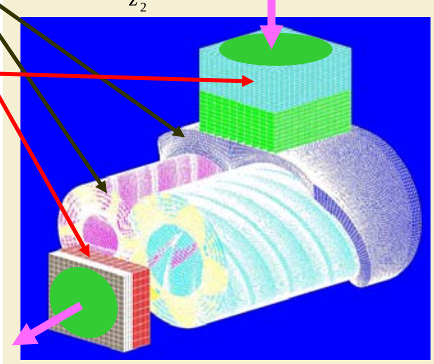
$$\dot{m}_{add} = \rho_i \frac{V_i}{p_i}\frac{\partial p_i}{\delta t} \approx \frac{p_{const} - p}{p_{const}} \cdot \frac{V\rho}{\delta t}$$

$$\dot{Q}_{add} = \dot{m}_{add} \cdot h_{add}$$

$$\int_V S_{c_i} dV = \rho \frac{\partial c_i}{\partial t} V_i = \dot{m}_i$$

$$\omega_1 = \frac{2n\pi}{60}; \qquad \mathbf{v}_{1i} = \mathbf{r}_{1i}\,\omega_1$$

$$\omega_2 = -\omega_1 \frac{z_1}{z_2}; \qquad \mathbf{v}_{2i} = \mathbf{r}_{2i}\,\omega_2$$



- Novel boundary conditions – boundary regions:
  Inlet & outlet receivers and oil port are treated as boundary domains

Multiphase flow

Liquid injection, Two phase expansion

-Euler-Lagrangian approach - continuous phase occupies entire domain, other phases dispersed in the first one

Common grid; One set of equations for continuous phase; Additional concentration equation for dispersed phase; Energy, mass & momentum sources

Momentum source

$$\frac{d(m_o \mathbf{v}_o)}{dt} = \mathbf{f}_{drag} + \mathbf{f}_{pres} + \mathbf{f}_{body} + \mathbf{f}_{am}$$

Energy balance for a dispersed phase

$$\frac{d(m_i h_i)}{dt} = m_o C_{p_o} \frac{dT_o}{dt} + h_L \frac{dm_L}{dt} = \dot{Q}_{con} + \dot{Q}_{mass}$$

Convective heat flux Heat flux with mass interch.

Energy source

$$\dot{Q}_{con} = \pi d_o \kappa \, \mathrm{Nu} (T - T_o) \qquad \dot{Q}_{mass} = h_L \frac{m_L - m_L^{\ s}}{\delta t} = h_L \dot{m}_L$$

Mass exchanged between phases

$$\dot{m}_L = \frac{dm_L}{dt} \approx \frac{\Delta m_L}{\delta t} = \frac{m_L - m_L^{\ s}}{\delta t}$$

Thermodynamic properties of real fluids

- *Ideal fluids* . . . .

$$u = f(T) \quad \rho = f(p,T) \quad u \neq f(p)$$
$$p/\rho = RT$$

- *Real fluids* . . . .

In any p-v-T equation for real fluids, only pressure is defined explicitly
All other variables are then calculated by an iterative procedure

- *p-v-T* equation compressibility factor *z*

$$p/\rho = z \cdot RT = z(p,T) \cdot RT$$

- *z* is assumed to change linearly with pressure err<2%

$$z = p \cdot B_1 + B_2$$

- Antoine equation for saturation temperature

$$T_{sat} = \frac{A_2}{A_1 - \log p} - A_3$$

- Clapeyron equation for latent heat

$$h_L = T_{sat} \cdot \left(\frac{1}{\rho_v} - \frac{1}{\rho_l} \right) \cdot \frac{dP_{sat}}{dT_{sat}}$$

- Coefficient in the pressure correction equation

$$C_\rho = \left(\frac{d\rho}{dp} \right)_T = \frac{1}{RT}$$

Integral Parameters

- Volume flow (inlet and outlet)

$$\dot{V} = 60 \cdot \sum_{t=t_{start}}^{t_{end}} \dot{V}_f^{(t)} \; \left[m^3/\min \right], \quad \dot{V}_f^{(t)} = \sum_{i=1}^{I} v_{fi} S_{fi}$$

- Mass flow (inlet, outlet, oil)

$$\dot{m} = \sum_{t=t_{start}}^{t_{end}} \dot{V}_f^{(t)} \cdot \bar{\rho}^{(t)} \; \left[kg/\sec \right]$$

- Boundary forces

$$F_x = p_b * A_{xb}; \quad F_y = p_b * A_{yb}; \quad F_z = p_b * A_{zb}$$

- Restraint Forces and Torque

$$F_{rS} = \sum_{i=1}^{I} F_{rS}(i),[N]; \quad F_{rD} = \sum_{i=1}^{I} F_{rD}(i), [N]$$

$$F_a = \sum_{i=1}^{I} F_a(i),[N]; \quad T = \sum_{i=1}^{I} T(i), [Nm]$$

- Compressor shaft power

$$P = 2 \cdot \pi \cdot n \cdot (T_M + T_F) \quad [W]$$

- Specific power

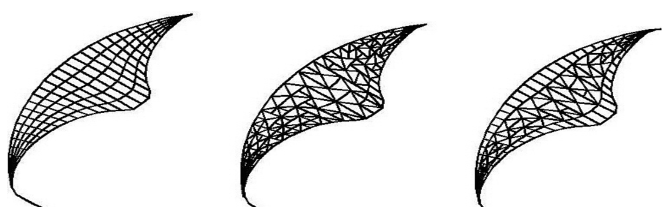
$$P_{spec} = P/\dot{V} \cdot 1000 \quad \left[kW/m^3 \min \right]$$

- Efficiency
  Volumetric and adiabatic

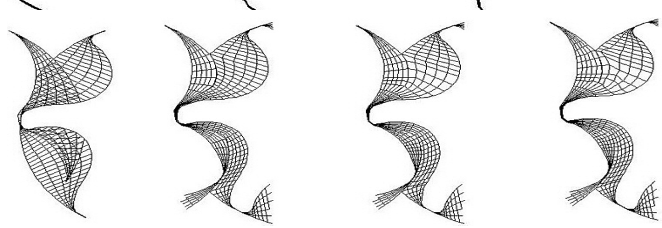
$$\eta_v = \dot{V}/V_d; \qquad \eta_i = P_{ad}/P$$

Grid generation

- Grid systems
  - structured
  - unstructured
  - mixed



- Block structured
  - discontinuous
  - continuous



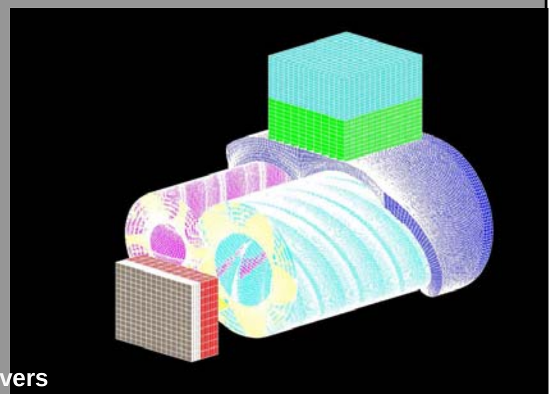
- Grid generation methods
  - Algebraic - interpolation or some special functions
  - Differential - based on the solution of partial differential equations
  - Variational - based on optimization of the grid quality properties.

Grid generation — Blocks

- Grid topology strongly affects accuracy, efficiency and ease of calculation
- Fully structured block generated hexahedral 3D-O mesh
- Screw compressor sub-domains are:
  - **Male rotor**
  - **Female rotor**
  - **End clearances**

These together contain all
Rotor connections
Clearances
Leakage paths

  - **Suction port**
  - **Discharge port**
  - **Suction and discharge receivers**



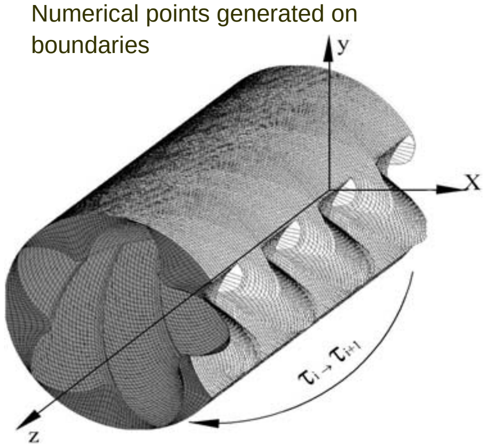
Grid generation

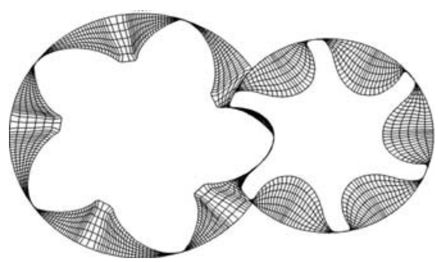
Rotor profiles generated from a rack

Rotors closed by a number of lobes

The rack connected to an outer circle

Numerical points generated on boundaries





Boundary point distribution adapted upon compressor's geometrical requirements

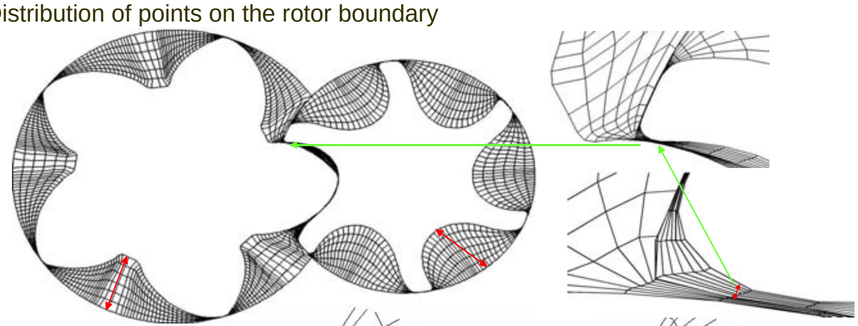
Inner grid points generated for 2-D structured "O" mesh

Same procedure repeated for all required cross sections of the grid

Same number of vertices in each cross section

Points on boundaries - adaptation

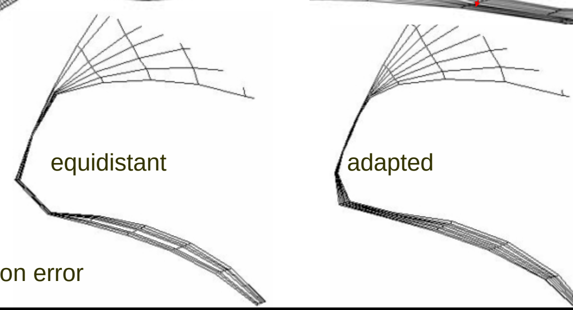
- Distribution of points on the rotor boundary



Equidistribution method

$$X_{\xi} \cdot W = const.$$

X_{ξ} - grid spacing
W – weight function



minimisation of the distribution error

Points on boundaries – adaptation 1

When integrated with the respect of a natural coordinate (arc-length)

$$\xi(s) = \int_0^s W(s)ds \Big/ \int_0^{S\max} W(s)ds$$

Weight function

$$W(s) = 1 + \sum_{i=1}^{I} b^i f^i(s)$$

Adaptation function
- tangent angle
- curve flatness
- centre distance
- radius of curvature
- sinusoidal & cosine distribution

$$F^i(s) = \int_0^S f^i(s)ds$$

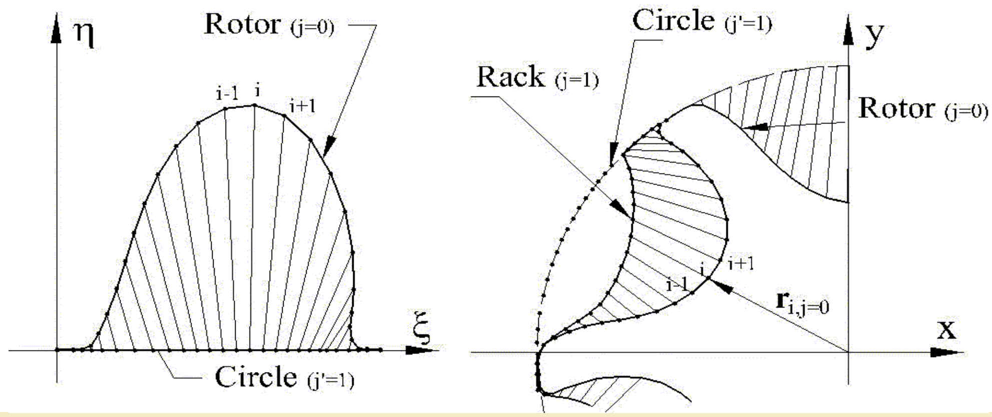
Grid point ratio

$$R^j = b^j F^j(S_{\max}) \Big/ \left\{ S_{\max} + \sum_{i=1}^{I} b^i F^i(S_{\max}) \right\}$$

Adaptation equation – final form:

$$\boxed{\xi(s) = \frac{s}{S_{\max}} \left\{ 1 - \sum_{i=1}^{I} R^i \right\} + \sum_{i=1}^{I} \left\{ R^i \frac{F^i(s)}{F^i(S_{\max})} \right\}}$$

Points on boundaries - distribution



$$\mathbf{r}_{i,j'=1} = \mathbf{r}_{i,j'=1}(x,y) = \mathbf{r}_{i,j'=1}\left(\frac{s_i}{s_I}\right) \qquad k_i = \frac{\eta'_i}{\zeta_i}$$

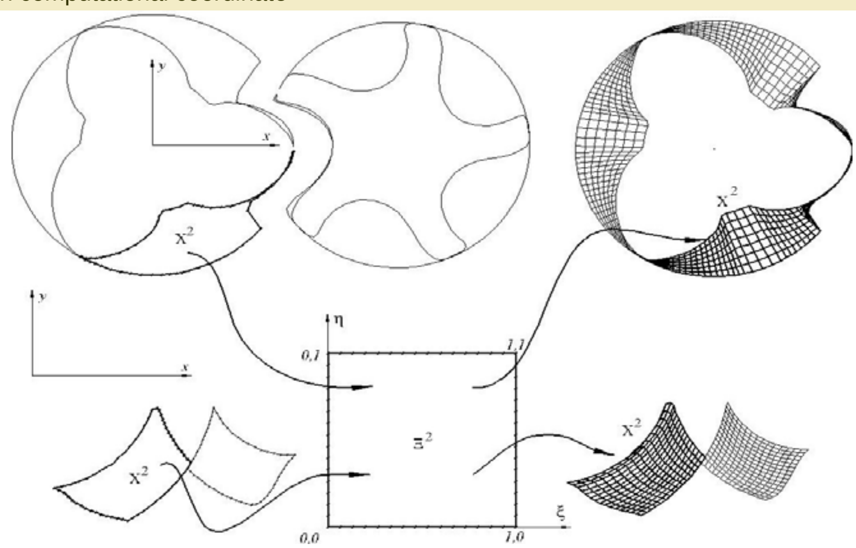
$$\xi_{i,j=0} = \xi_{i-1,j=0} + c\,\cos\alpha_{ac};\; \xi_{i,j'=1} = \xi_{i,j=0}$$

$$\eta_{i,j=0} = c\sin\alpha_{ac}; \qquad \eta_{i,j'=1} = 0$$

$$\mathbf{r}^*_{i,j'=1} = \mathbf{r}^*_{i,j'=1}(x,y) = \mathbf{r}_{I,j'=1}\left(\frac{\xi^*_i}{\xi^*_I}\right)$$

Transfinite interpolation

Multivariate interpolation procedure or a Boolean sum of univariate interpolations along each computational coordinate



Transfinite interpolation – Lagrange 1

Standard formula of transfinite interpolation:

$$\mathbf{r}_1(\xi,\eta) = \sum_{l=1}^{2} \alpha_l(\xi)\mathbf{a}_l(\eta)$$

$$\mathbf{r}\ (\xi,\eta) = \mathbf{r}_1(\xi,\eta) + \sum_{l=1}^{2} \beta_l(\eta)[\mathbf{b}_l(\xi) - \mathbf{r}_1(\xi,\eta_l)]\ ,$$

$$\mathbf{a}_l(\eta) = \mathbf{r}(\xi_l,\eta)$$
$$\mathbf{b}_l(\xi) = \mathbf{r}(\xi\ ,\eta_l)$$

Boundary points

$$\alpha_l(\xi_k) = \delta_{kl}$$
$$\beta_l(\eta_k) = \delta_{kl}$$
$$k=1,2;\ l=1,2$$

Restriction for blending functions

Coordinates of internal points in 2D domain:

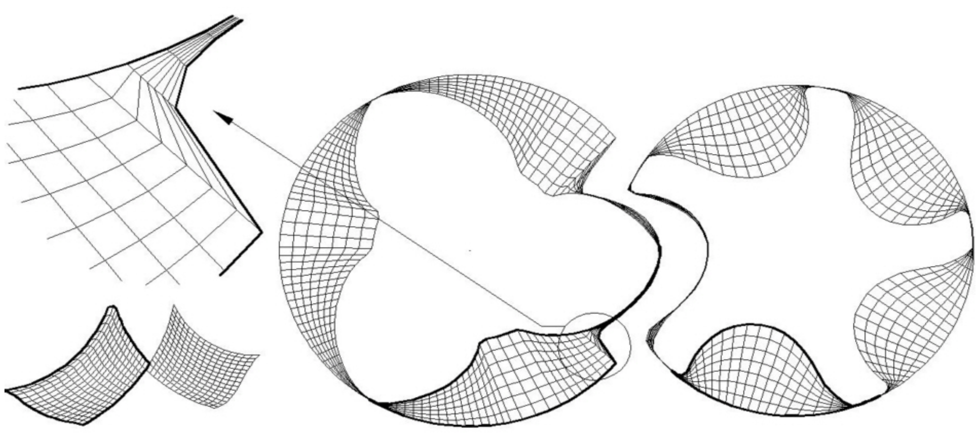
$$\boxed{\begin{aligned} x(\xi,\eta) &= X_1(\xi,\eta)\alpha_1(\xi) + X_2(\xi,\eta)\alpha_2(\xi) \\ y(\xi,\eta) &= Y_1(\xi,\eta)\beta_1(\eta) + Y_2(\xi,\eta)\beta_2(\eta) \end{aligned}}$$

Lagrange functions:

$$\alpha_1(\bar{\xi}) = 1 - \bar{\xi},\ \alpha_2(\bar{\xi}) = \bar{\xi}$$
$$\beta_1(\bar{\eta}) = 1 - \bar{\eta},\ \beta_2(\bar{\eta}) = \bar{\eta}$$

- Fast method applicable for simple grids.
- Orthogonality is not achieved except for the most simple grids.
- Can be used only as the initial grid for further orthogonalisation and smoothing

Transfinite interpolation – Lagrange 2



a) Outlet port

b) Rotors

Transfinite interpolation – Hermite 1

Ortho formula of transfinite interpolation:

$$\mathbf{r}_1(\xi,\eta) = \sum_{l=1}^{2}\sum_{n=0}^{1} \alpha_l{}^n(\xi)\mathbf{a}_l{}^n(\eta)$$

$$\mathbf{r}\ (\xi,\eta) = \mathbf{r}_1(\xi,\eta) + \sum_{l=1}^{2}\sum_{n=0}^{1} \beta_l{}^n(\eta)[\mathbf{b}_l{}^n(\xi) - \frac{\partial^n}{\partial\eta^n}\mathbf{r}_1(\xi,\eta_l)]\ ,$$

Boundary points and derivatives:

$$\mathbf{a}_l{}^n(\eta) = \frac{\partial^n}{\partial\xi^n}\mathbf{r}(\xi_l,\eta)$$

$$\mathbf{b}_l{}^n(\xi) = \frac{\partial^n}{\partial\eta^n}\mathbf{r}(\xi\ ,\eta_l)$$

Restriction for blending functions:

$$\frac{\partial^n}{\partial\xi^n}\alpha_l{}^n(\xi_k) = \delta_{kl}\delta_{nm}$$

$$\frac{\partial^n}{\partial\eta^n}\beta_l{}^n(\eta_k) = \delta_{kl}\delta_{nm} \qquad k=1,2;\ l=1,2;\ n=0,1;\ m=0,1$$

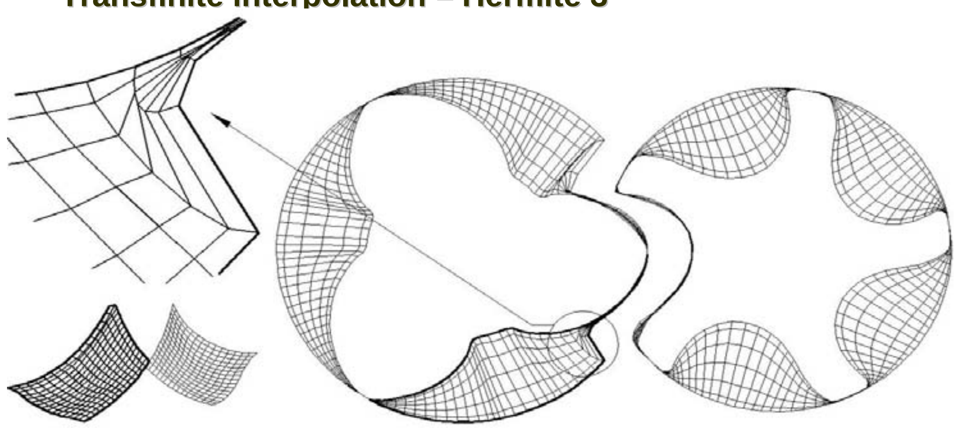
Coordinates of internal points in 2D domain :

$$\boxed{\begin{aligned} x(\xi,\eta) &= x'(\xi,\eta) + \Delta x(\xi,\eta) \\ y(\xi,\eta) &= y'(\xi,\eta) + \Delta y(\xi,\eta) \end{aligned}}$$

Hermite blending functions:

$$\alpha_1^0 = h_1(\eta) = 2\eta^3 - 3\eta^2 + 1$$
$$\alpha_1^1 = h_2(\eta) = -2\eta^3 + 3\eta^2$$
$$\alpha_2^0 = h_3(\eta) = \eta^3 - 2\eta^2 + \eta$$
$$\alpha_2^1 = h_4(\eta) = \eta^3 - \eta^2$$

Transfinite interpolation – Hermite 3

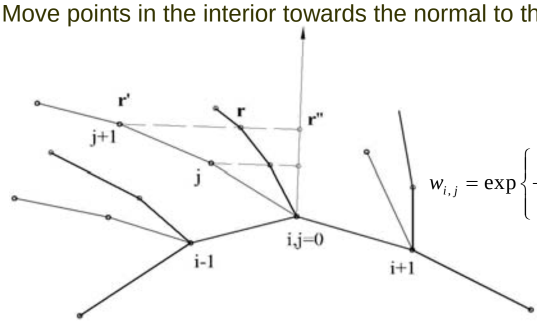


a) Outlet port b) Rotors

- Much more complex then Lagrange interpolation. Requires user's attention!
- Gives orthogonal and regular meshes for simpler domains (Ports)
- Overlapping and irregularities for complex domains with discontinuities

Transfinite interpolation – Orthogonalisation 1

Generate regular, not necessarily orthogonal mesh.
Move points in the interior towards the normal to the boundary



$$\boxed{\mathbf{r}_{i,j} = (1-w_{i,j})\mathbf{r}'_{i,j} + w_{i,j}\mathbf{r}''_{i,j}}$$

$$w_{i,j} = \exp\left\{-C_1\left[\left(1-\frac{\tilde{\eta}_{i,j}}{\tilde{\eta}_{i,j_{\max}}}\right)-1\right]\right\}\cdot\left[4\xi_{i,0}(1-\xi_{i,0})\right]^{C_2}$$

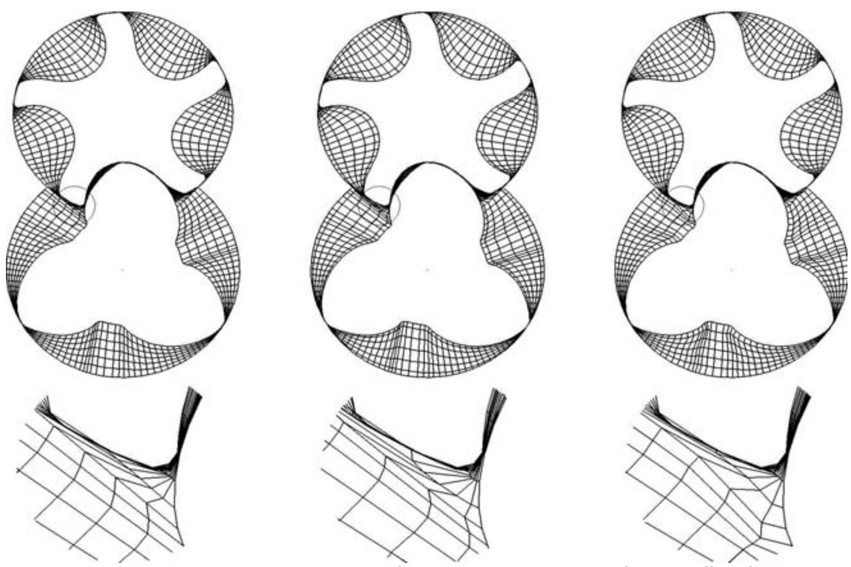
$$\tilde{\eta}_{i,j} = \sqrt{(\xi_{i,j}-\xi_{i,0})^2+(\eta_{i,j}-\eta_{i,0})^2}$$

Grid smoothing

$$x_{i,j}^{n+1} = x_{i,j}^{n} + C\left(x_{i+1,j}^{n} - 2x_{i,j}^{n} + x_{i-1,j}^{n}\right)$$

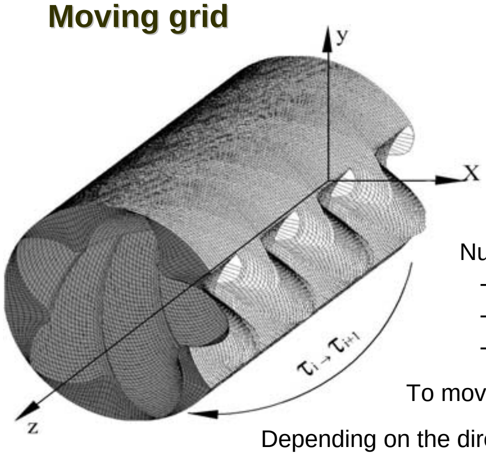
$$y_{i,j}^{n+1} = y_{i,j}^{n} + C\left(y_{i+1,j}^{n} - 2y_{i,j}^{n} + y_{i-1,j}^{n}\right), \quad C \le 0.5,\ n = 0,1,\dots,N$$

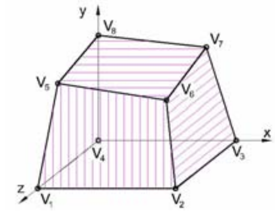
Transfinite interpolation – Orthogonalisation 2



Lagrange | Hermite | Orthogonalised Lagrange

Moving grid





Numerical grid usually defined by:
- Cell definition: CellNo + 8xVertNo
- Vertex definit.: VertNo + 3Coord.
- Region defin: RegNo + 4xVertNo

To move grid – redefine vertices

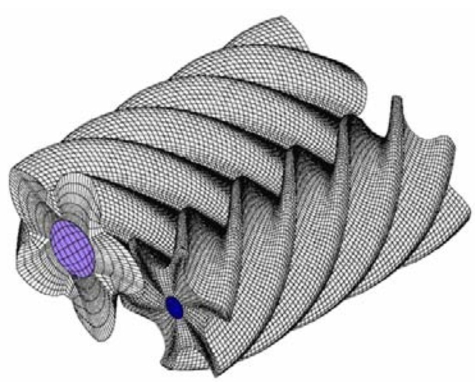
Depending on the direction of rotation move all layers for

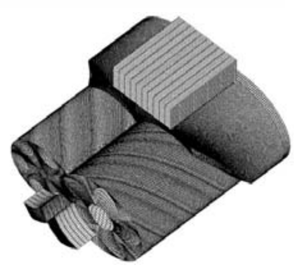
$$\Delta z = L / z_1 n_{ang}$$

And assign appropriate coordinate position to each vertex in each layer.

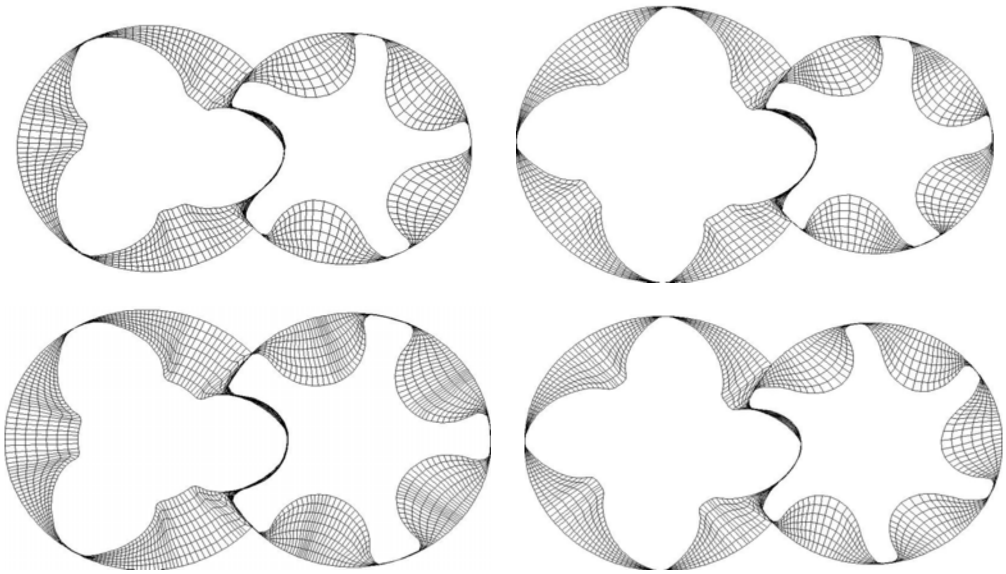
By this means, in each time step rotors are rotated for: $$\delta\varphi = \frac{2\pi}{z_1 n_{ang}}$$

Moving grid generated by SCORG

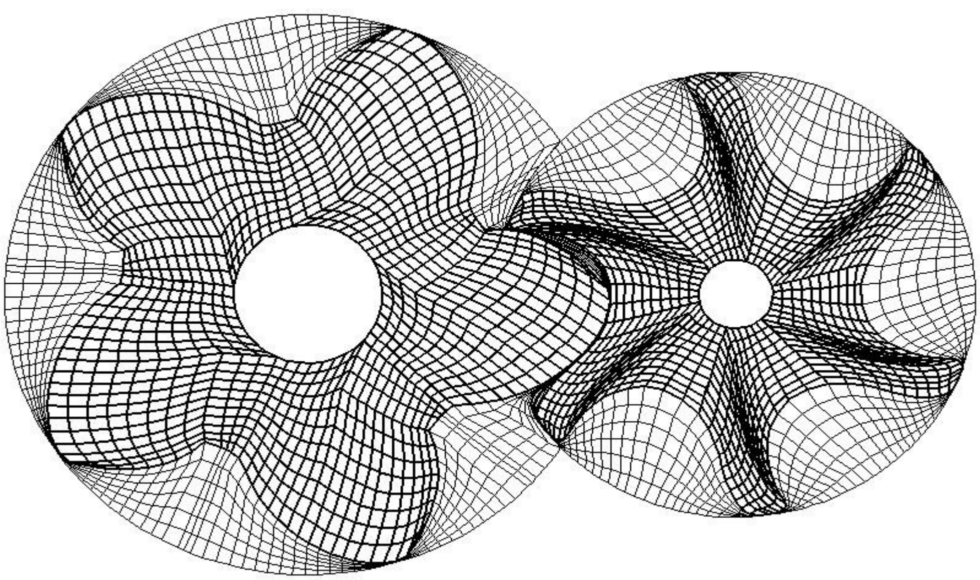


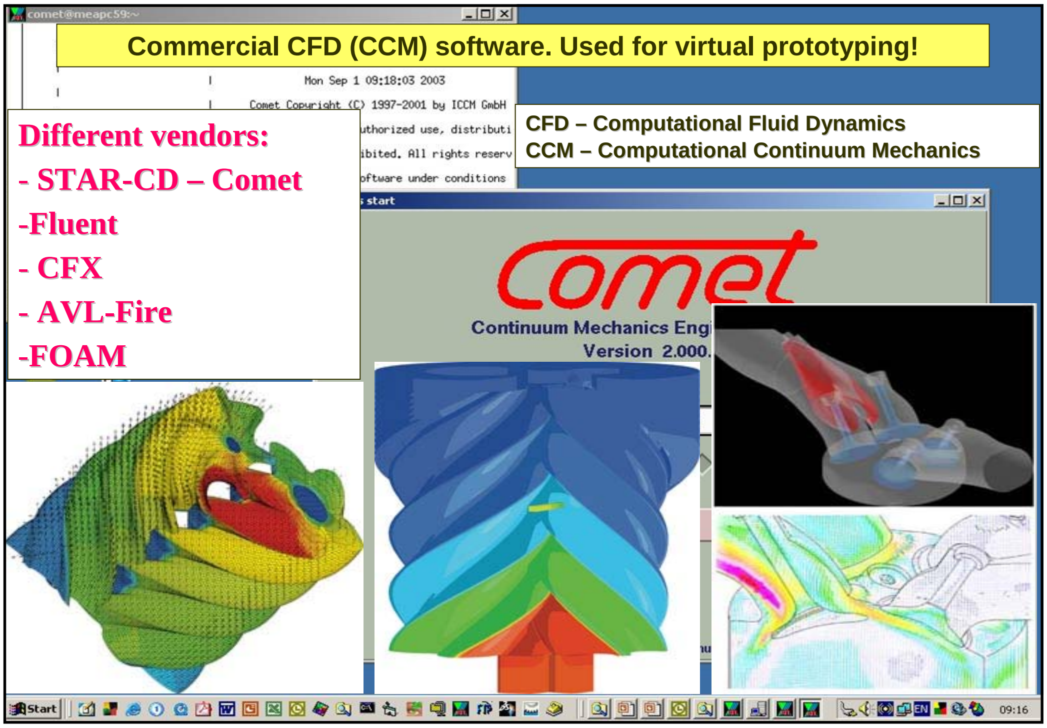


Examples – Profiles



Examples – Influence of the mesh size

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