Resolution limits of continuous media models and their mathematical formulations

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Grand Challenge – Exaflops Computations

- Supercomputers performance gain – 1 exaFLOPS – 2018
- Sufficiently wide usage of 1 petaFLOPS systems – 2015
- Real need for high-performance computing: oil and gas recovery and optimization, ecologically save combustion, nuclear and fusion, turbulence, astrophysics

- Current state: relatively small number of simulations using > 100 TFLOPS
- Practically, 100 TFLOPS barrier exists
- Reason: Lack of mathematical models, numerical algorithms and software well suitable for high-performance computers
- Need for logically simple yet efficient algorithms for modern hardware architectures
- Solution by means of fundamental science
- This problem in principle does not depend on the type of used computer (CPU or GPGPU).

For adaptation we need logically simple **but effective algorithms**. And usually these two features are opposite – this is the main problem.

Explicit schemes give rise to the logically simple algorithms. But they have strong time step restrictions for the stability reason.

For the hyperbolic type of equation:

$$\Delta t \le h \qquad (1)$$

where Δt is time step, h is character space step

For the parabolic type of equation:

$$\Delta t \le h^2 \qquad (2)$$

The condition (2) practically does not give the opportunity to use very fine space meshes.

- “Physically” infinitesimal volume contains several tens of molecules
- For air at normal conditions characteristic space scale is $l^{*} \sim 10^{-6} \mathrm{cm}$

$$l_0 \ll l^* \ll l$$

l_0 – size of molecule 10^{-8} cm,

l – free path length $l^{*} \sim 10^{-4} \mathrm{cm}$

- Heat equation –

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} K \frac{\partial T}{\partial x} + I$$

paradox of instantaneous heat propagation

- Implicit scheme – paradox exists

$$\frac{T_i^{j+1} - T_i^j}{\Delta t} = K\frac{T_{i+1}^{j+1} - 2T_i^{j+1} + T_{i-1}^{j+1}}{\Delta x^2} + I$$

- Explicit scheme – finite propagation speed

$$\frac{T_i^{j+1} - T_i^j}{\Delta t} = K\frac{T_{i+1}^{j} - 2T_i^{j} + T_{i-1}^{j}}{\Delta x^2} + I$$

- Model of hyperbolic heat conduction:

$$\frac{\partial T}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 T}{\partial t^2} = \frac{\partial}{\partial x}K\frac{\partial T}{\partial x} + I$$

$$\Delta t \gtrsim \tau \qquad \tau^* \sim 10^{-8}\ \text{sec}$$

$$\Delta t \leq \frac{\Delta x^2}{2K}, \quad \Delta t \sim \tau = \frac{l}{c}, \quad K \sim l \cdot c \qquad \Delta x \gtrsim l$$

- Kinetic schemes – quasi gas-dynamic system (QGS) - 1983

$$f(x, \zeta, t^{j+1})$$

$$t^{j+1} = t^j + \tau$$

$$f_0(x - \zeta\tau, \zeta, t^j)$$

$$f\left(\bar{x}, \bar{\zeta}, t^{j+1}\right) = f_0(\bar{x} - \bar{\zeta}\tau, \bar{\zeta}, t^{j+1}) \qquad \frac{l}{L} \ll 1$$

$$f^{j+1} - f^j = -\tau\zeta_i \frac{\partial f_0}{\partial x_i} + \frac{\partial}{\partial x_i} \frac{\tau^2}{2} \zeta_i \zeta_k \frac{\partial f_0}{\partial x_k} \qquad \frac{|\zeta|\tau}{L} \ll 1$$

- Multiply by summatoric invariants

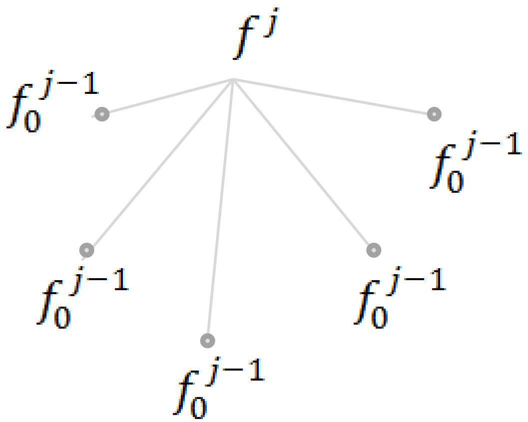
$$1, \bar{\zeta}, {\zeta^2}/{2}$$

and integrate over range of molecules velocities

Lattice Boltzmann schemes

- Bhatnagar-Gross-Krook (BGK) model:

$$\frac{df}{dt} = \nu(f_0 - f)$$



$$\rho = \sum f^j \Delta\zeta$$

$$\rho U = \sum f^j \zeta \Delta\zeta$$

- Explicit schemes:

  The role of free path length plays *h*

$$Re = \frac{\rho U L}{\mu} \qquad \mu \sim lc \cdot \rho$$

Hyperbolic system – QGS

$$\frac{\partial \rho}{\partial t} + \tau \frac{\partial^2 \rho}{\partial t^2} + \frac{\partial \rho U}{\partial x} = \frac{\partial}{\partial x}\frac{\tau}{2}\frac{\partial}{\partial x}(\rho U^2 + P), \qquad \tau = \frac{\mu}{P}$$

$$\frac{\partial \rho U}{\partial t} + \tau \frac{\partial^2 \rho U}{\partial t^2} + \frac{\partial}{\partial x}(\rho U^2 + P) = \frac{\partial}{\partial x}\frac{\tau}{2}\frac{\partial}{\partial x}(\rho U^3 + 3PU)$$

$$\frac{\partial E}{\partial t} + \tau \frac{\partial^2 E}{\partial t^2} + \frac{\partial}{\partial x}\big(U(E+P)\big) = \frac{\partial}{\partial x}\frac{\tau}{2}\frac{\partial}{\partial x}(U^2(E+2P) + \frac{\partial}{\partial x}\frac{\tau}{2}\frac{\partial}{\partial x}\left[\frac{P}{\rho}(E+P)\right]$$

QGS =N-S + O(Kn^2)

QGS – alternative Navier-Stokes

QGS – was used for simulation of many problems:

DNS-turbulence, unsteady flows, aeroacoustic,

incompressible fluid, combustion phenomena

Combustion Flows

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial^2 \rho_i}{\partial t^2} + \frac{\partial \rho_i U}{\partial x} = \frac{\partial}{\partial x}\frac{\tau}{2}\frac{\partial}{\partial x}\left(\rho_i U^2 + P_i\right) \quad - \text{ self diffusion}$$

$i = 1 \ldots N - 1$, $\quad i$ – number of species

$\rho = \rho_i, \qquad P = P_i$

$$\frac{\partial}{\rho \partial t} + \frac{\partial^2}{\rho \partial t^2} + \frac{\partial \rho U}{\partial x} = \frac{\partial}{\partial x}\frac{\tau}{2}\frac{\partial}{\partial x}\left(\rho\, U^2 + P\right) \quad \rightarrow \quad O(\mathrm{Kn}^2)$$

$$\frac{\partial \rho U}{\partial t} + \frac{\partial^2 \rho U}{\partial t^2} + \frac{\partial U^2 + P}{\partial x} = \frac{\partial}{\partial x}\frac{\tau}{2}\frac{\partial}{\partial x}\left(\rho\, U^3 + 3PU\right)$$

$$\frac{\partial T}{\partial t} + \frac{\tau^*}{2}\frac{\partial^2 T}{\partial t^2} = \frac{\partial}{\partial x} K \frac{\partial^2 T}{\partial x^2} + I$$

$$\left[\tau^* \frac{\partial^2 T}{\partial t^2}\right] \ll \left[\frac{\partial T}{\partial t}\right]$$

$$\tau^* \sim {}^{h}/_{c}$$

$$\frac{T_i^{j+1} - T_i^{j-1}}{2\Delta t} + \frac{\tau^*}{2}\frac{T_i^{j+1} - 2T_i^j + T_i^{j+1}}{\Delta t^2} = K\frac{T_{i-1}^j - 2T_i^j + T_{i+1}^j}{\Delta x^2}$$

$$\frac{\tau^*}{2\Delta t^2} = \frac{K}{\Delta x^2}$$ - Dufort-Frankel Method $\Delta t \sim h^{3/2}$

$$\Delta t \sim h$$

$$\frac{\partial U}{\partial t} - divA\nabla U = f$$

A **– symmetric matrix**

$$\delta \frac{\partial^2 U^\delta}{\partial t^2} + \frac{\partial U^\delta}{\partial t} - divA\nabla U^\delta = f$$

$$\delta \geq \varepsilon > 0$$

$$e = U^\delta - U \ \ , t\epsilon[0,T]$$

$$\int_\Omega \int_0^T \|\nabla e\|^2 \, dtdx + \int_\Omega |e(x,T)|^2 \, dx \leq \delta^2 C_1 \int_0^T \int_\Omega \left|\frac{\partial^2 U^\delta}{\partial t^2}\right|^2 dxdt$$

Stabilizing corrections method

$$-U\frac{d\Phi}{dx}+K\frac{d^2\Phi}{dx^2}+Q=0$$

- Integrating over $x_b - x_a = h$ and using Taylor expansion:

$$-U\frac{d\Phi}{dx}+K\frac{d^2\Phi}{dx^2}+Q+\frac{h}{2}\frac{d}{dx}U\frac{d\Phi}{dx}=0$$

$\tau^* = {}^{h}/_{U}$ - “internal” time

$$-U\frac{d\Phi}{dx}+K\frac{d^2\Phi}{dx^2}+Q+\frac{d}{dx}\frac{\tau^*}{2}\frac{d\Phi \mathrm{U}^2}{dx}=0$$

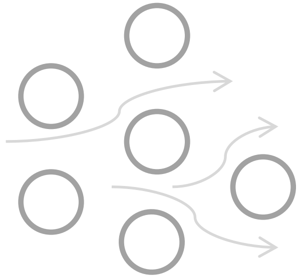
- Given enough computational power, detalization level (value *h*) is defined by practice requirements

Filtration problems

$$\frac{\partial \rho}{\partial t} + div \rho \overline{U} = 0 \quad (1)$$

$$KU = -grad\ P \quad (2)$$

$$\rho = \rho_0 [1 + \beta (P - \rho_0)] \quad (3)$$



$$\frac{\partial \rho}{\partial t} + \tau^* \frac{\partial^2 \rho}{\partial t^2} + div \rho U = div \frac{\tilde{l} c}{2} grad\ \rho$$

$\tilde{l} \ll L$ - geology size

$$KU = -grad\ P$$

$\hat{l}$ - several tens of rock grains

$$\rho = \rho_0 [1 + \beta (P - \rho_0)]$$

Boltzmann equation

$$\frac{\partial f}{\partial t} + \zeta \frac{\partial f}{\partial x} = J(f, f')$$

$$\frac{f_i^{j+1} - f_i^j}{\Delta t} + \zeta \frac{f_{i+1}^j - f_{i-1}^j}{2\Delta x} = \frac{|\zeta|\Delta x}{2} \frac{f_{i+1}^j - 2f_i^j + f_{i-1}^j}{(\Delta x)^2} + J(f, f')$$

$$\frac{\partial f}{\partial t} + \tau^* \frac{\partial^2 f}{\partial t^2} + \zeta \frac{\partial f}{\partial x} = \frac{|\zeta| l^*}{2} \frac{\partial^2 f}{\partial x^2} + J(f, f')$$

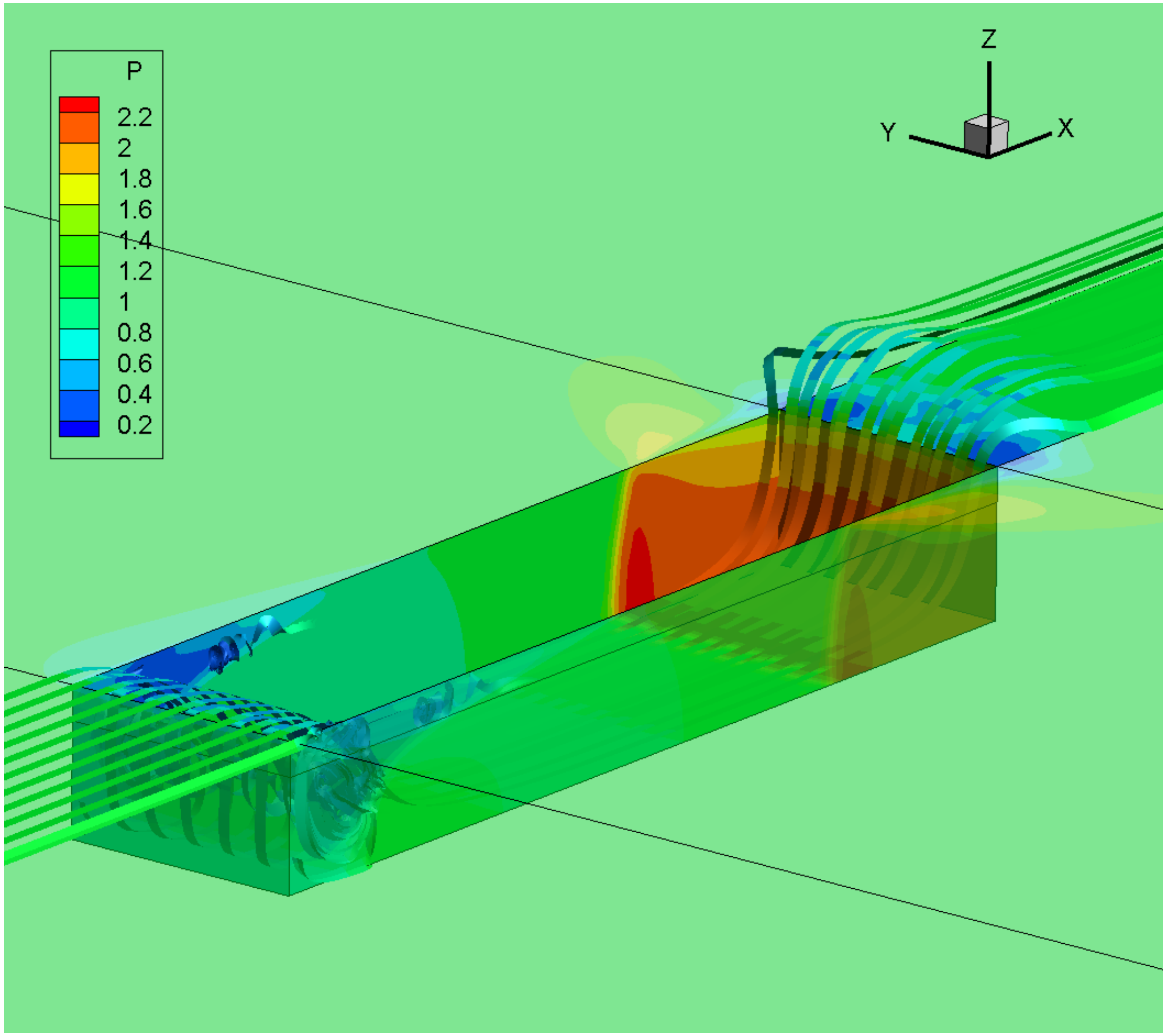
$\tau^* - l_0/c \quad - 10^{-14}$ sec $\qquad l_0 \sim 10^{-8}$ cm

f - has probabilistic character , volume of diameter l^* has to contain several tens of molecules

$$l_0 \ll l^* \ll l$$

$$\frac{\partial f}{\partial t} + \zeta \frac{\partial f}{\partial x} = \frac{1}{2} \frac{\partial}{\partial x} |\zeta| l^* \frac{\partial f}{\partial x} + J(f, f')$$

Flow in cavity simulation



$4.5 \cdot 10^9$ mesh nodes
GPGPU “Lomonosov”
Efficiency 68.1%
1200 Tesla cards

Streamlines and pressure level sets

Hyperbolic Model of Multiphase Fluid Flow in Porous Medium

$$m\frac{\partial(\rho_\alpha S_\alpha)}{\partial t}+\tau\frac{\partial^2(\rho_\alpha S_\alpha)}{\partial t^2}+\mathrm{div}(\rho_\alpha \mathbf{u}_\alpha)=$$

$$=q_\alpha+\mathrm{div}\frac{l_\alpha c_\alpha}{2}\mathrm{grad}(\rho_\alpha S_\alpha)$$

$$\mathbf{u}_\alpha=-K\frac{k_\alpha}{\mu_\alpha}(\mathrm{grad}\,p_\alpha-\rho_\alpha\mathbf{g})$$

$$\rho_\alpha=\rho_{0\alpha}\left[1+\beta_\alpha\left(p_\alpha-p_{0\alpha}\right)\right]$$

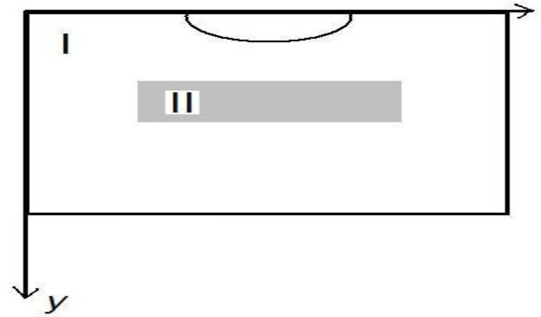
$$\sum_\alpha S_\alpha=1$$

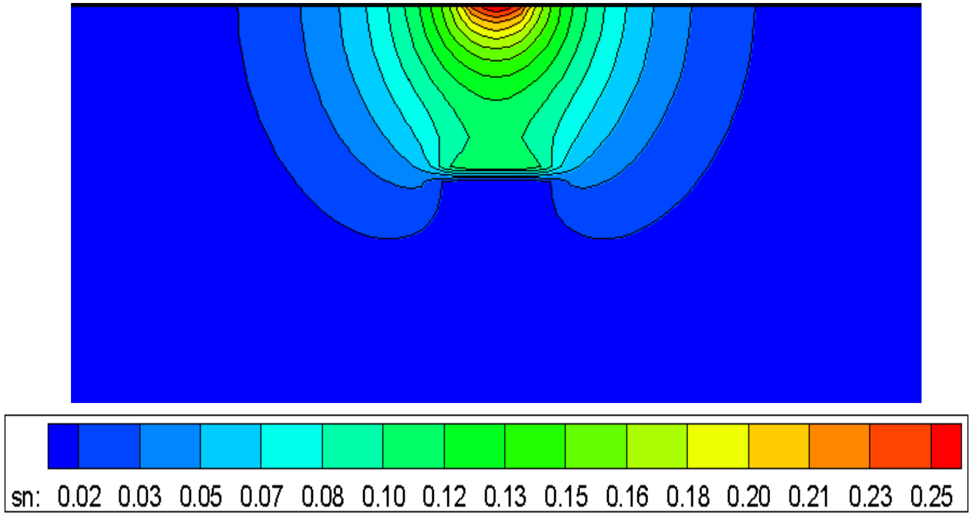
$$p_\alpha-p_\beta=p_{c\,\alpha\beta}(S_\alpha,S_\beta),\quad \alpha\neq\beta$$

$\alpha\ (\beta)$ indicates the phase

$$\Delta t \le h^{3/2}$$

3D problem of tetrachloroethylene infiltration into the water-saturated soil (vertical central section)





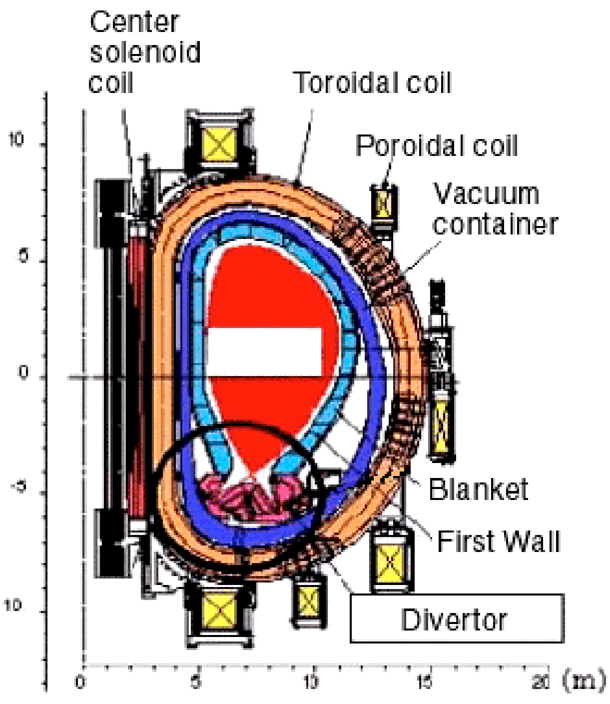
$1.5\cdot10^9$ mesh nodes

K-100 - 100TFLOPs

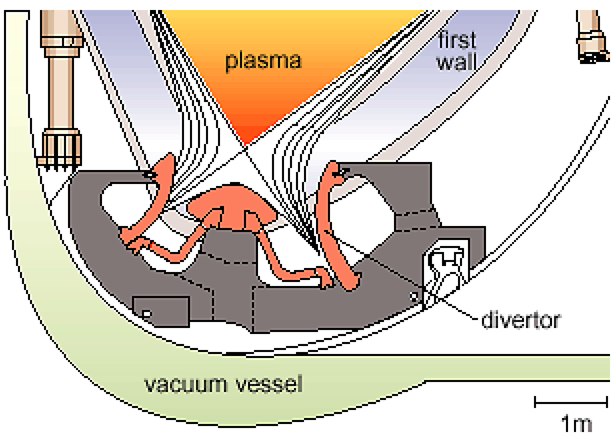
Contaminant saturation field

The immediate task is the development of the model for turbulent heat and mass transfer in ITER divertor (MHD + turbulence + radiative transfer).

Cross-section of ITER

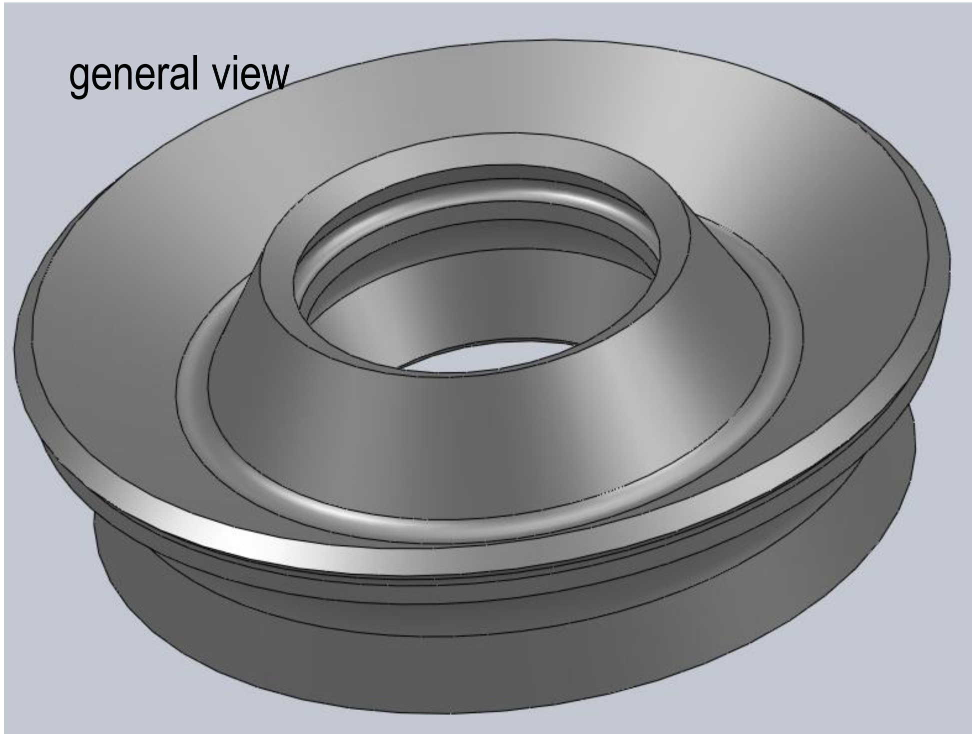


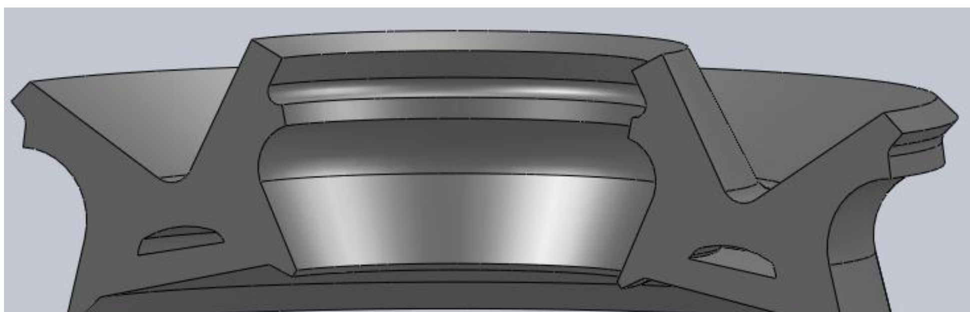
Magnified view of divertor area



CAD images

general view

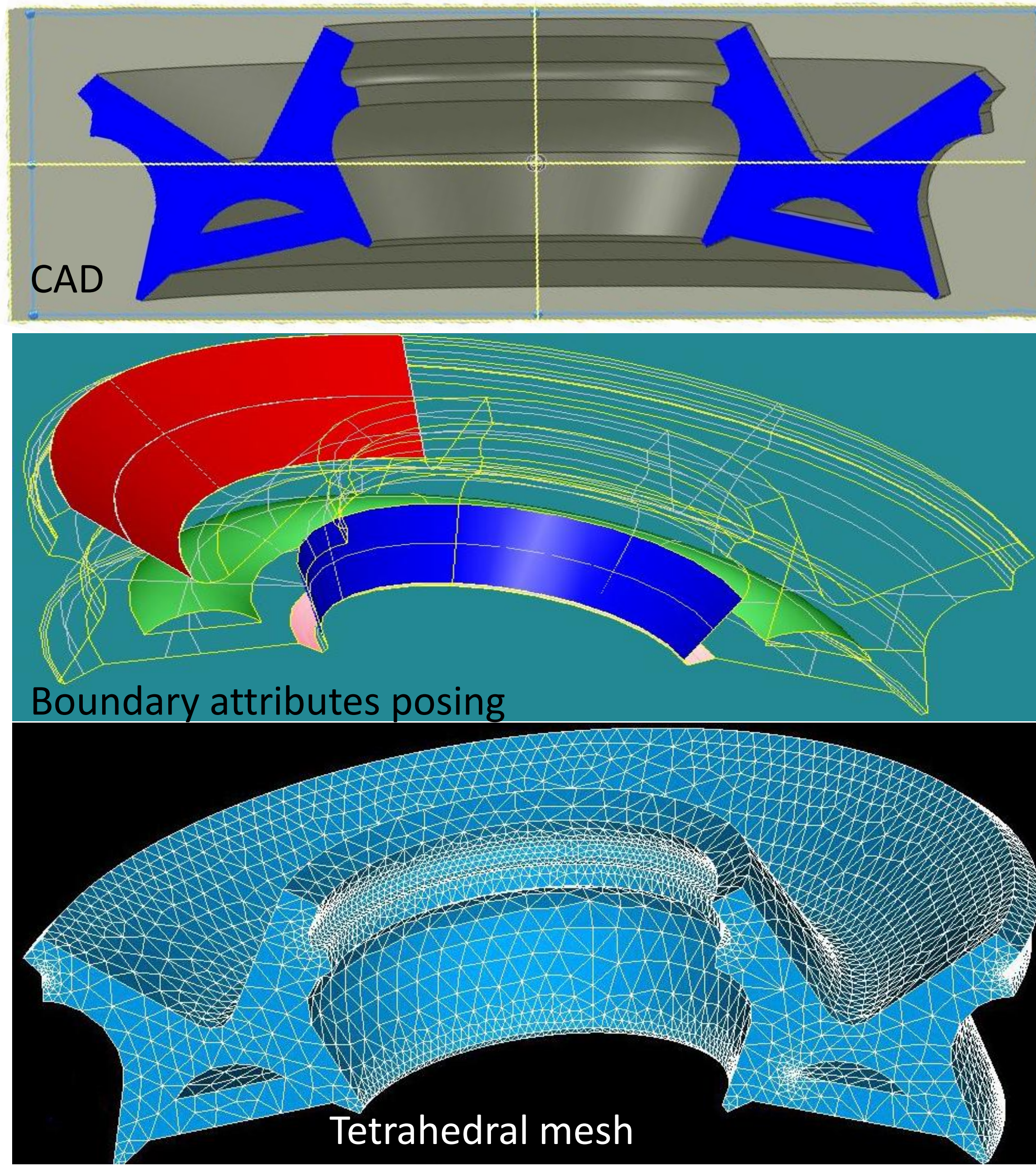




cross-section

Turbulent heat and mass transfer in ITER divertor:

From CAD model
to computational mesh



Initial tetrahedral mesh before refinement is shown.
The resulting mesh includes 10^8 cells and more.

Kinetic schemes and QGS for MHD

$$f_0 = \frac{\rho}{(2\pi KT)^{3/2}} \exp\left\{-\left(\bar{\xi} - \bar{U}(x,t) - i\bar{w}\right)\right\}^2$$

$$w = \frac{\bar{B}}{\sqrt{\rho}} \qquad \varphi = \left(1, \xi, \frac{\xi^2}{2}, i\xi^2\right)$$

$$\rho = \int f_0 d\xi, \quad \bar{U} = \frac{1}{\rho}\int \xi f d\xi, \quad E = \int \frac{\xi^2}{2} f_0 d\xi$$

$$B = -\frac{1}{\sqrt{\rho}} \int m\xi^* f_0 d\xi$$

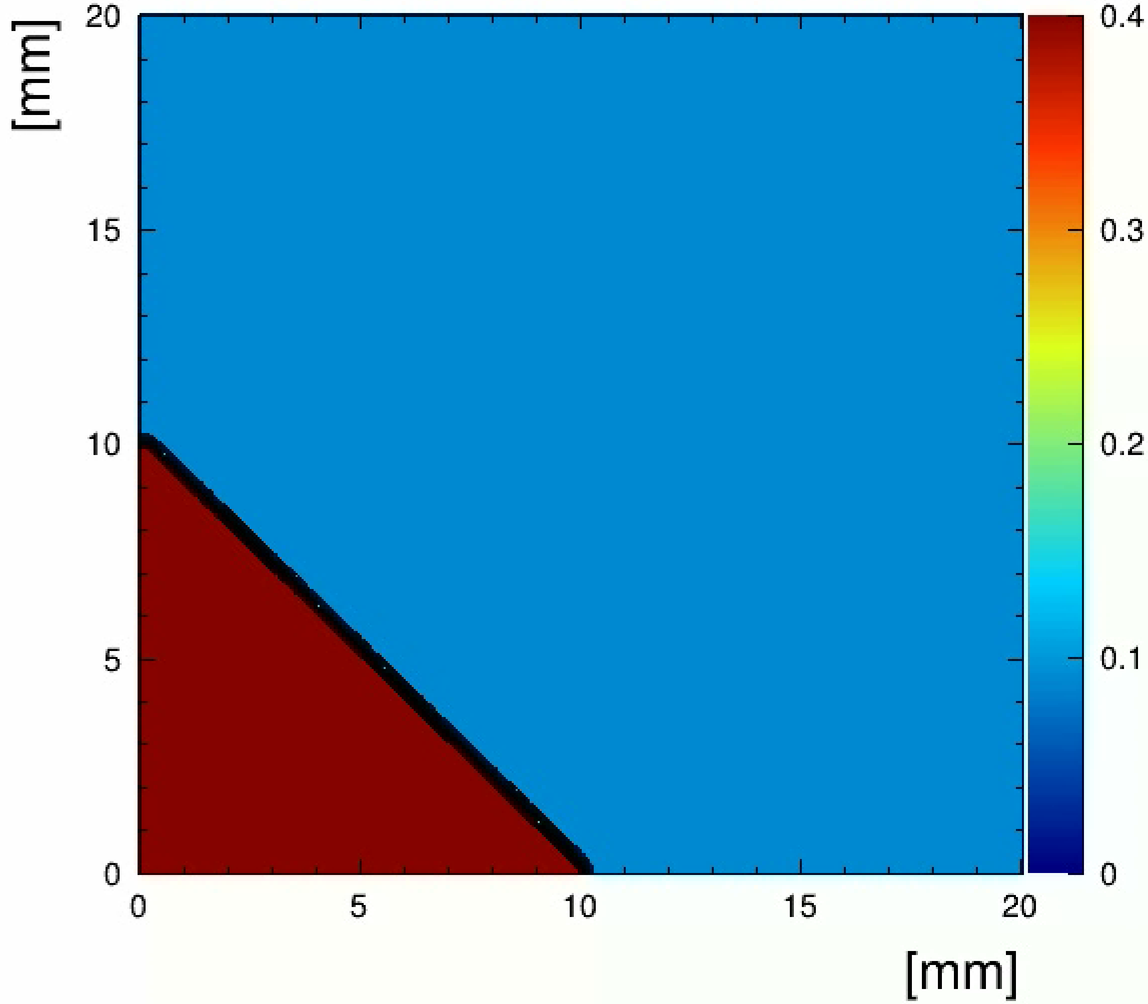
$$\int f d\xi \quad \times \quad \frac{\partial \rho}{\partial t} + \frac{\partial \rho U_K}{\partial x_K} = 0$$

$$\int f\xi d\xi \quad \times \quad \frac{\partial \rho U_K}{\partial t} + \frac{\partial}{\partial x_K}\left[\left(P + \frac{B^2}{2}\right)\delta_{PK} + \rho U_{KP} - B_K B_P\right] = 0$$

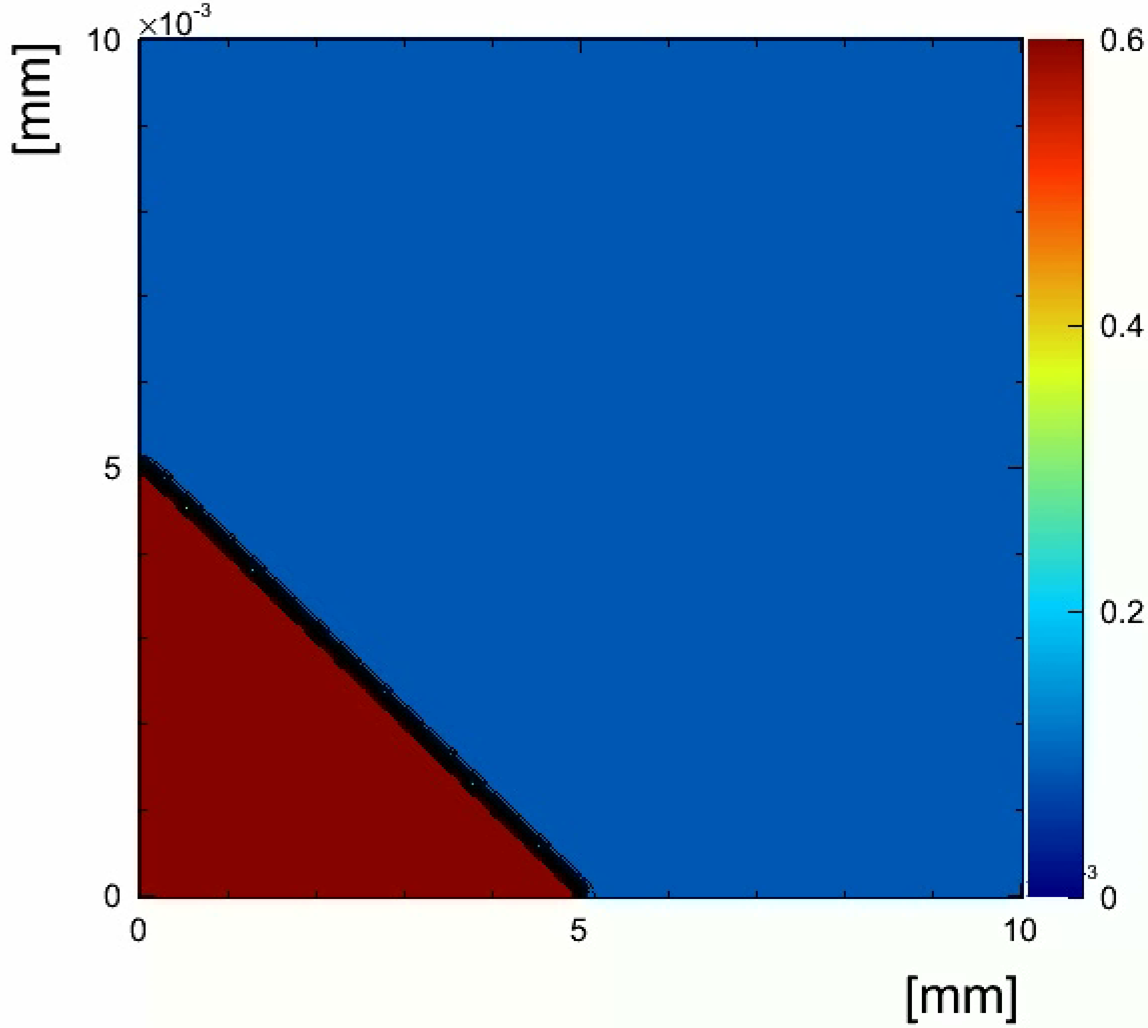
$$\int f \frac{\xi^2}{2} d\xi \quad \times \quad \frac{\partial E}{\partial t} + \frac{\partial}{\partial x_K}\left[U_K\left(E + P + \frac{B^2}{2}\right) - B_K \sum_P U_i B_P\right] = 0$$

$$\int f i\xi^* d\xi \quad \times \quad \frac{\partial B_K}{\partial t} - \frac{\partial}{\partial x_K}\left[U_P B_K - U_K B_P\right] = 0$$

$$\frac{\partial B_K}{\partial x_K} = 0 \qquad , \tau, \qquad \tau_m$$



[mm]
20
15
10
5
0
0
5
10
15
20
[mm]
0.4
0.3
0.2
0.1
0



[mm]
×10^-3
10
5
0
0
5
10
[mm]
0.6
0.4
0.2
0

[redacted]

Conclusions

- For some problems, modern computers don't pose any constraints on solution detalization level
- There exists natural space scales, such that further detalization have no real sense
- Additional terms, usually, have a form of physically motivated regularizer which smooth out non-physical numerical effects
- Numerical values of the involved regularization coefficients has to be known up to the order of magnitude
- Using such regularizators we get opportunity to adapt algorithms on the architecture of extra massive parallel computer systems

References

1. B.N.Chetverushkin. Kinetic schemes and qusigasdynamic system of equations. Barselona. CIMNE. 2008 (in English).
2. B.N.Chetverushkin. Resolution Limits of Continuous Media Models and their Mathematical Formulations. Matematicheskoye Modelirovanie. 2012. №11 (in Russian). Mathematical Models and Computer Simulations. 2013. V.5, №3, pp.266-279 (in English).